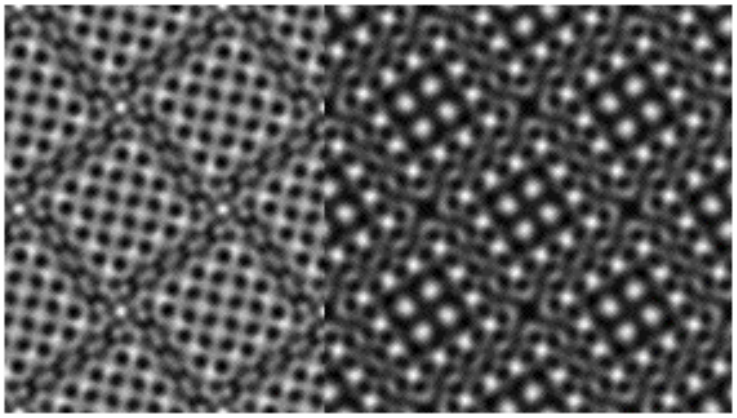
V4.0

xHREM™

(WinHREM™/MacHREM™)

High Resolution Electron Microscope Simulation Suite

User's Guide



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Support/Update

Email: support@hremresearch.com
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Getting Started

In this chapter
we explain the concept of xHREM™
and how to install them.
Then, you will learn how to use xHREM™
by using the attached examples.

■ Introduction

High Resolution Electron Microscopy (HREM) becomes an indispensable tool for understanding material properties or evaluating new materials at the level of atomic resolution. Due to increased demands for research and development of the new materials, an image simulation acquires more importance than ever before.

xHREM™ (WinHREM™ /MacHREM™) is a suite of the high-resolution electron microscope image simulation programs that will run on Windows or Mac OS.

Concept of xHREM™

1. User Friendly Graphical Interface

   xHREM™ employs user friendly Data Generation Utilities based on the Graphical User Interface for Windows or Mac OS.

   xHREM™ is general-purpose software that can be used to simulate all the images expected from any crystal systems, defect structures and interfaces. Although data generation for such general-purpose software normally becomes complex, a novice user can easily generate his/her data by using the graphical Data Generation Utilities with minimum requirements for the special knowledge.

2. Reliable and Efficient Algorithm

   Since electron microscope images critically depend on an electron-specimen interaction as well as aberrations of image forming lenses, the treatment of scattering based on dynamical theory and the treatment of aberration based on wave-optical theory are mandatory.

   xHREM™ emerges from the HREM image simulation programs based

on FFT multislice technique developed at Arizona State University, USA (see References). This is one of the most reliable and efficient HREM image simulation programs.

3. High Quality Image Output

Numerical data such as projected potential, wave function propagating the specimen, simulated image intensities could printed as high quality gray scale maps (Bitmap) by using Output Graphic Utilities. Numerical value of each pixel of the gray scale can be exported for further analysis with other software.

Features of *xHREM ™*

- Efficient algorithm based on Fast Fourier Transform (FFT)
- Applicable to any crystal systems and symmetries for an arbitrary beam direction
- Applicable to defects, interfaces and artificial supper-lattices
- Treatment of partial coherency based on the transmission cross-coefficient
- Coherent Convergent Beam Electron Diffraction (Option)
- High resolution STEM image simulation including HAADF-STEM images (Option)

Steps for Image Simulation with xHREM™

xHREM™ consists of three graphical user interfaces (GUI) for scattering calculation, image intensity calculation and scattering intensity output. There are also other utilities for half-tone (gray-scale) image outputs. Even a novice user can easily generate input data satisfying the format required by the calculation programs, and then execute calculations. High quality simulated images are easily obtained by using the gray-scale output utilities.

Each GUI uses a window, called WORKSHEET, to assist the user to fill out the necessary data. When saving (Save or Save As…) the input data in the WORKSHEET, the GUI converts the WORKSHEET data into the input data required by the calculation program. Actual calculation is easily performed from the menu command (Execute) by using the converted data.

To get gray-scale microscope images do the followings:

1. Generate a required data for scattering calculation by using the

graphical user interface called MultiGUI, and then perform calculation from Execute command of the File menu.

2. Generate a required data for image calculation by using the graphical user interface called ImageGUI, and then perform calculation from Execute command of the File menu.
3. Obtain gray-scale images from the calculated images by using the utility called ImageBMP. The output gray-scale images may be arranged into a table layout (Image Tableau) as functions of thickness and defocus.

References

K. Ishizuka and N. Uyeda: A New Theoretical and Practical Approach to the Multislice Method, Acta Cryst. A33 (1977) 740-749.

K. Ishizuka: Contrast Transfer of Crystal Images in TEM, Ultramicroscopy 5 (1980) 55-65

K. Ishizuka: Multislice Formula for Inclined Illumination, Acta Cryst. A38 (1982) 773-779.

K. Ishizuka: A practical approach for STEM image simulation based on the FFT multislice method, Ultramicroscopy 90 (2001) 71-83.

■ Before using xHREM™

If you are not familiar with routine operations of Windows/Mac OS such as a clicking, double-clicking or dragging the mouse, a menu selection, a file open/close procedure and so on, please consult the user's manual come with your computer for getting acquainted with Window GUI before using xHREM™ .

■ Installation

Installing for Windows

xHREM (WinHREM™) is distributed on-line. The software should be installed into the hard disk by following the standard procedure below.

Unzip the downloaded file, and execute 'Setup.exe' by double-clicking it. It is advised that the WinHREM programs are installed into the directory named 'xHREM' under /Program Files/HREM Research as instructed by the installer.

The structure of the 'xHREM' folder on the hard disk will be the one shown below. Sample data will be installed in the 'xHREM Data' folder under your ‘My Documents’ directory.

The installer will register WinHREM application icons (shortcuts) under 'xHREM' on the Start menu.

Installing for Mac OS X

xHREM (MacHREM™) is distributed on-line. The software should be installed into the hard disk by following the standard procedure below.

Open a disk image file (.dmg) that you have downloaded. Then, in order to install the program, open xHREM.pkg and select xHREM (English) or xHREM (Japanese). Next, install the data using Data.pkg.

The structure of the 'xHREM' folder on the hard disk will be the one shown below.

The structure of xHREM program folder

Utilities	: GUI, Output Utilities
Programs	: Programs for numerical calculation
Resources	: Resources used by Utilities
Documents	: Manuals

How to use 64bit version

The programs for 64bit version are already installed by the above installation process. However, by default the 32bit version programs have been selected. In order to use the 64bit programs please select “64bit” from Execution mode of the Preferences.

(Windows) Installing User Key Driver

Installing User Key Driver

NOTE: Disconnect the USB key.

Launch "HASPUserSetup.exe," and follow the instructions to install the user key driver.

Installing User Key

Simply plug your USB key into an USB port.

If your user key is not recognized, the software will run as a demonstration version.

(Mac OS) Installing User Key Driver

Installing User Key Driver

NOTE: Disconnect the USB key.

Open the disk image file (.dmg) that you have downloaded, and follow the instructions to install the user key driver.

Installing User Key

Simply plug your USB key into an USB port.

If your user key is not recognized, the software will run as a demonstration version.

■ Let's Start Tutorials

How to use GUI for Data Input

By using three graphic user interfaces (GUIs), the required data for numerical calculations are prepared by filling the window called WORKSHEET. Each GUI has File, Edit and Help menus. Please consult the references for the details of each menu.

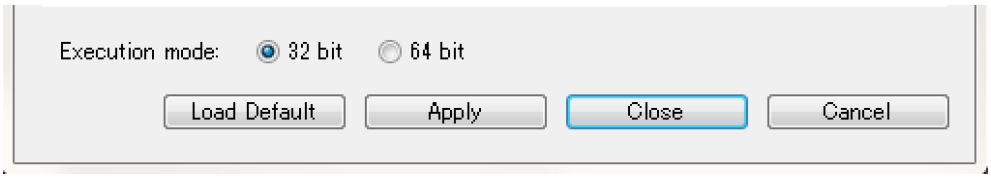
Example Data

Two sets of data are provided within the Data folder for exercises. They are a tin oxide (SnO_2) and a complex oxide of tungsten and niobium ($W_8Nb_{18}O_{89}$), and their sample name are SnO2 and WNbO, respectively. We use SnO2 here as an example, but the same steps can be applied to WNbO. Please play with WnbO by yourself later.

At first we calculate scatting amplitudes, and then calculate image intensities. The gray-scale images or diffraction patterns will be obtained from the image intensities of the scatting amplitudes.

How to use 64bit version

The programs for 64bit version are already installed by the above installation process. However, by default the 32bit version programs have been selected. In order to use the 64bit programs please select “64bit” from Execution mode of the Preferences.



Scattering Amplitude calculation

At first, let's prepare the data required for the scatting amplitude calculation:

1. Launch MultiGUI.

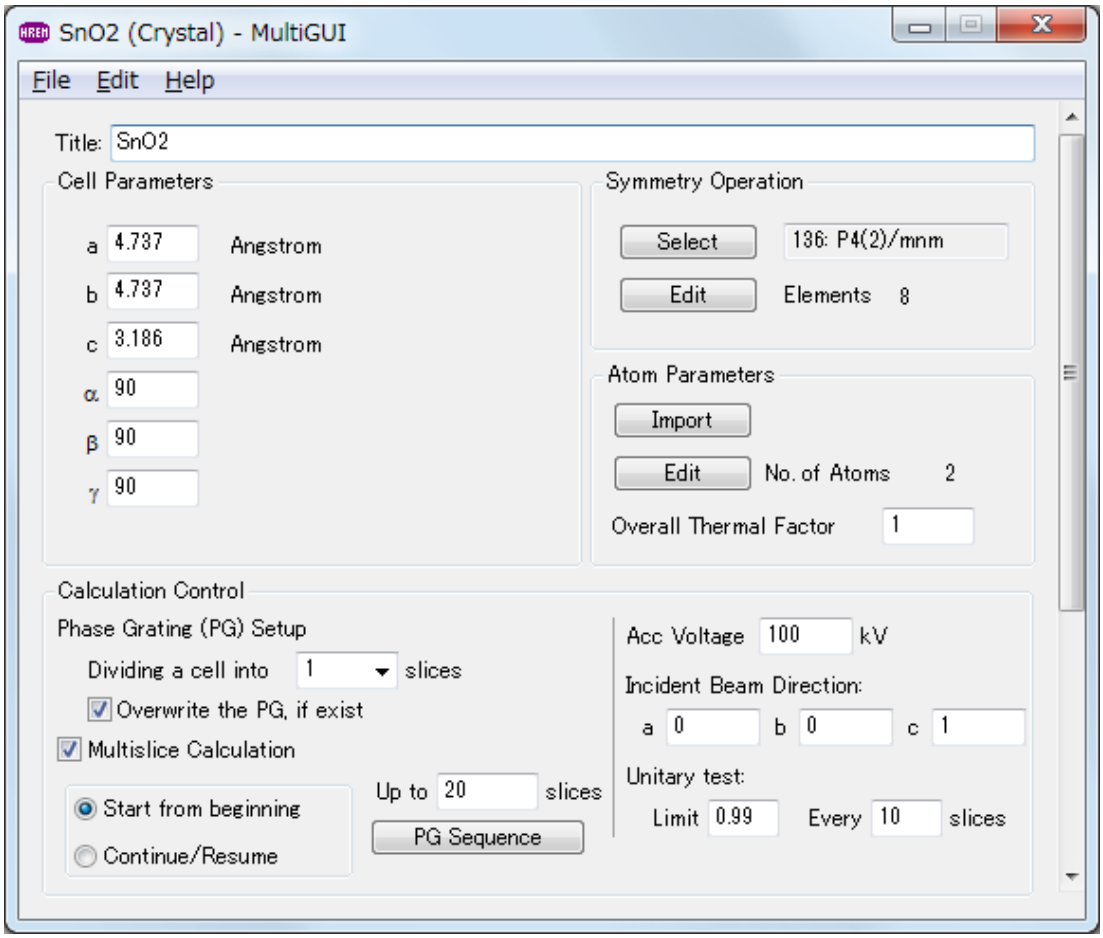
   Please consult your computer manual about how to launch an application.

2. Choose "Open..." from the File menu to browse the sample data, and select “SnO2.WS1”.

   Please consult your computer manual about how to select a file.

   The WORKSHEET for data input will appear.

TIPS: The lower part of the WORKSHEET can be accessed by sliding the window or by expanding the display area.



In this WORKSHEET, appropriate data is already filled out. Here, let's create a new data set by changing the Title entry:

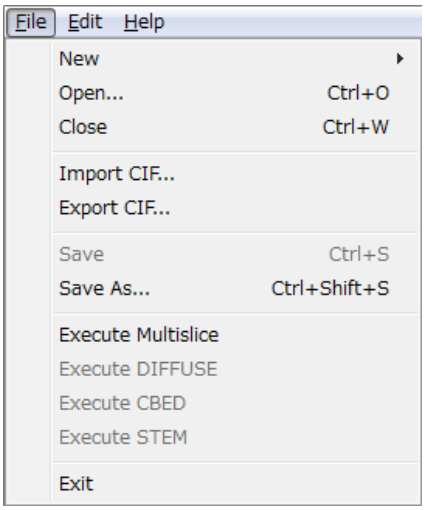
3. Input a new title "SnO2 test calculation" in the Title field.
4. Choose "Save As..." from the File menu.
5. Save the new data as "SnO2test" in the save dialog appeared.

   Please consult your computer manual about how to save your file.

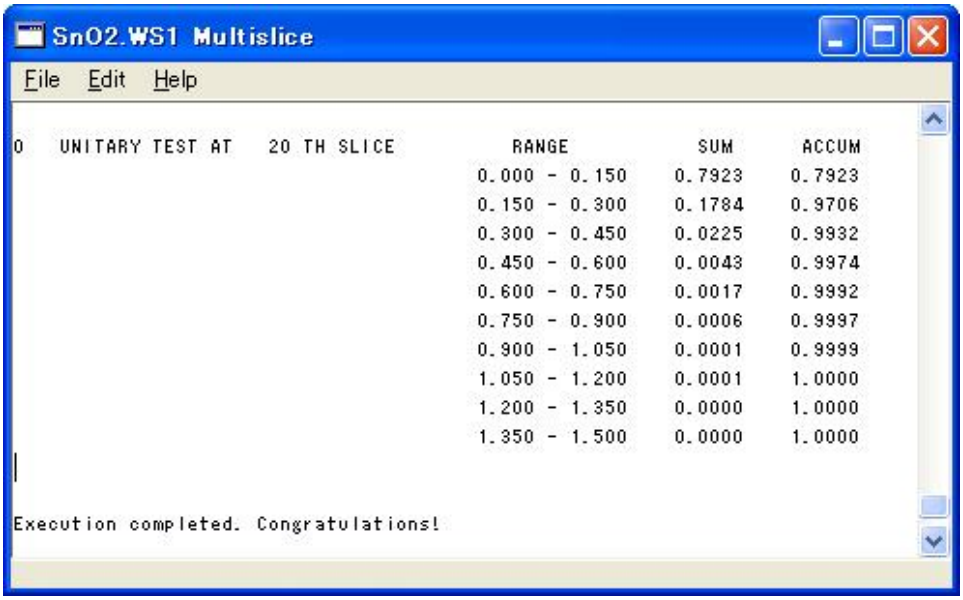
   TIPS: An extension '.WS1' will be added automatically. Thus, you may not need to specify the extension.

Next, we calculate the scattering amplitudes by using the data crested above:

6. Choose 'Execute Multislice' from File menu.



The program (multi.exe) that calculates the scattering amplitudes will be launched, and the progress of calculation will be displayed on a separate window. When an execution terminates normally, you will see the message "Execution completed. Congratulations!"



NOTE: The progress window has the fundamental menus such as File and Edit, and you can Save the content of the window from the File menu.

TIPS: The program can be terminated even in the middle of calculation by Exit command from the File menu or clicking the close button.

The progress window can be closed by Exit command from the File menu or clicking the close.

7. To terminate MultiGUI, select 'Exit(Quit)' from the File menu.

Image Intensity Calculation

The process for the image intensity calculation is similar with the scattering amplitude calculation. Before this step, you must prepare the scattering data (.DF) by using MultiGUI.

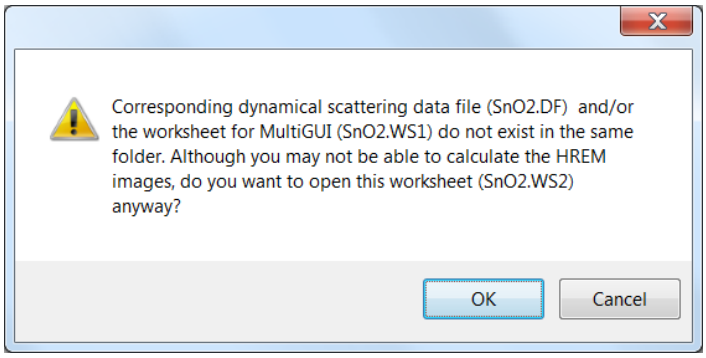
1. Launch ImageGUI.

   NOTE: There is no WS2 file corresponding to the data name that we have used for the MultiGUI, namely SnO2test.WS2. Thus, we will create it using an existing data (SnO2.WS2). You may create a WS2 data from a scratch by using Default.WS2.

2. Choose “Open…” from File menu to browse the worksheet (.WS2), and select SnO2.WS2 in the Data folder.

   Please consult your computer manual about how to select a file.

   NOTE: When you haven’t finished dynamical scattering calculation for SnO2 data, you will get the following warning message. Then, press “OK” and continue the steps.


Corresponding dynamical scattering data file (SnO2.DF) and/or the worksheet for MultiGUI (SnO2.WS1) do not exist in the same folder. Although you may not be able to calculate the HREM images, do you want to open this worksheet (SnO2.WS2) anyway?
OK
Cancel

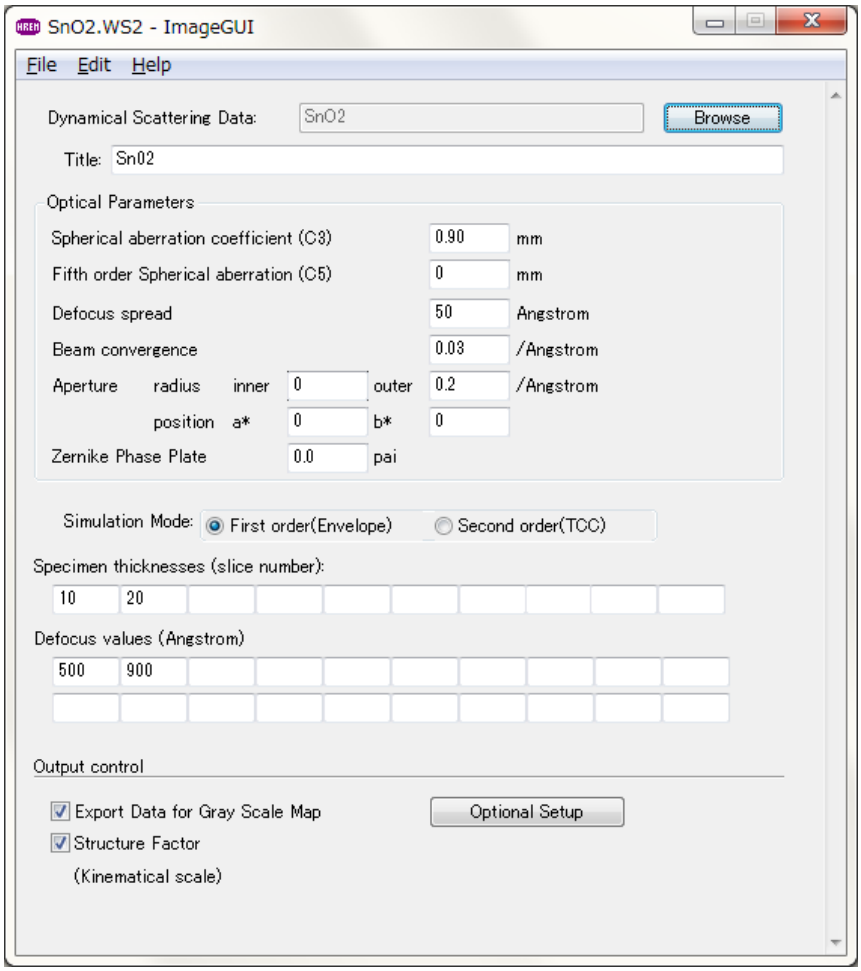
   The worksheet shown in the next page will be opened.

   TIPS: The lower part of the WORKSHEET can be accessed by sliding the window or by expanding the display area.

   In this WORKSHEET, appropriate data is already filled out. Here, let's create a new data set by changing the Dynamical Scattering Data:

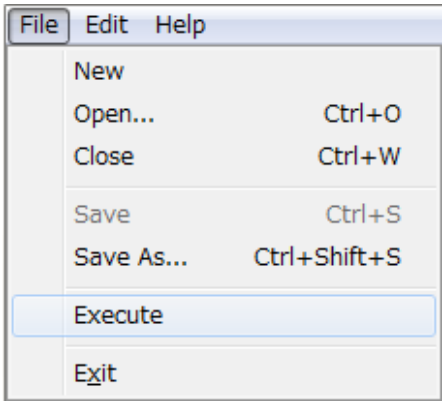
3. Using “Browse” button, select the data set “SnO2test.DF”.
4. Input a new title "SnO2 test calculation" in the Title field.
5. Choose "Save As..." from the File menu.
6. Save the new data as "SnO2test" in the save dialog appeared.

   TIPS An extension '.WS2' will be added automatically. Thus, you may not need to specify the extension.



Next, we calculate the image intensities by using the data crested above:

7. Choose 'Execute' from File menu.



The program (Image.exe) that calculates the image intensities will be launched, and the progress of calculation will be displayed on a separate

window. When an execution terminates normally, you will see the message "Execution completed. Congratulations!"

NOTE: The progress window has the fundamental menus such as File and Edit, and you can Save the content of the window from the File menu.

TIPS: The program can be terminated even in the middle of calculation by Exit command from the File menu or clicking the close button.

The progress window can be closed by Exit command from the File menu or clicking the close.

8. To terminate ImageGUI, select 'Exit(Quit)' from the File menu.

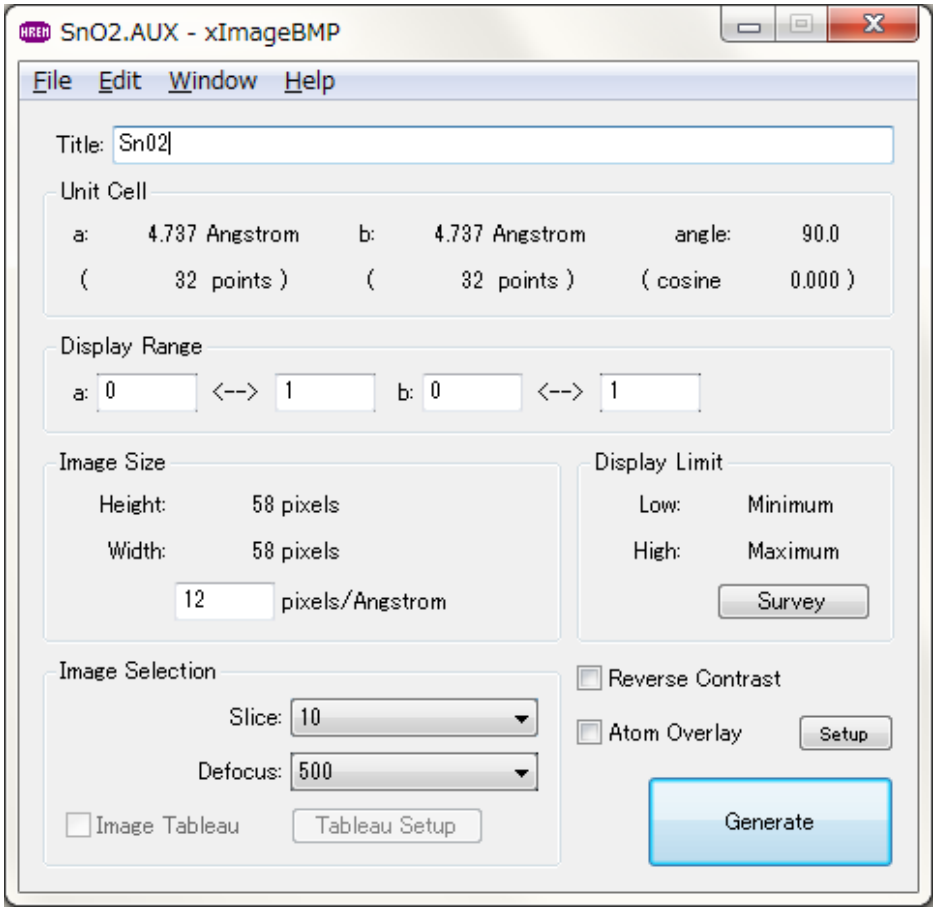
EM Image Display

Then, let's display gray-scale (half-tone) images that have been numerically calculated for SnO2 by using ImageGUI.

At first, you have to launch a utility and select a numerical image data to be displayed:

1. Launch ImageBMP.
2. A data selection dialog will be opened. Select SnO2test.AUX in the Data folder. (A data file for image display has ".AUX".)

   The following window will be appeared.



Then, let's get some images.

3. Click "Generate" in the right bottom of WORKSHEET.

   After a few seconds, you may get a gray-scale image shown below. This is an image calculated for the conditions corresponding to a slice and a defocus specified in the WORKSHEET. Specifically, Slice: 10; Defocus: 500 A (under-focus); Display Range: (0<->1) x (0<->1).

Next, draw a wider gray-scale image extended over a few unit cells.

4. Change end-points (left input-boxes) of a and b of "Display Range" to two (2).
5. Click "Generate" as before.

   You will get a gray-scale image of 2 x 2 unit cells as shown below.

6. You can save each gray-scale image by choosing "Save" or "Save As…" from "File" menu, if you want to.

   You can choose an image format in the dialog that will appear.

   If you want to save a quantitative data (binary data) of the displayed image, you can use "Export Data…" command (Please refer to Topics/Numarical Data Output using ImageBMP).

   You can also print each gray scale image by choosing "Print" from "File" menu.

7. Close each Bitmap window by choosing "Close" from "File" menu.

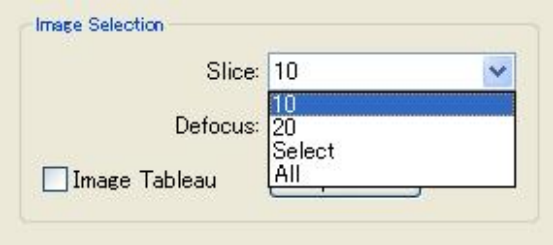
   If the gray-scale image has never been saved, a dialog for confirming your action.

   TIPS: You can avoid this confirmation dialog, when you close the window while pressing the "Shift" key.

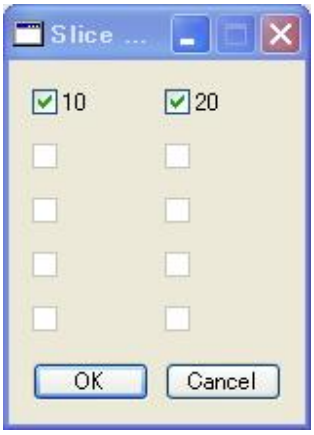
8. To terminate ImageBMP, select "Exit (Quit)" from "File" menu.

   NOTE: The default file name of an EM image is "Sample name_slice number_defocus.bmp."

To obtain an image at other slice and/or defocus, select a slice number and/or defocus value from the "Slice" and "Defocus" pull-down menus. These pull-down menus show all possible selections on your data set.



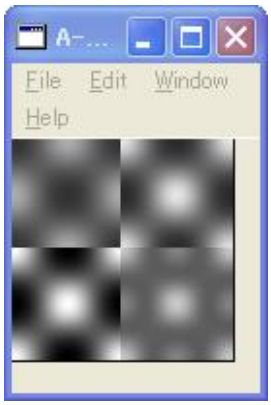
When you choose “Select” from “Slice” or “Defocus” pull-down menu, you will get a following dialog, where you can select the slices or defocuses that you want to display.



TIPS: If you choose "All" or “Select” from "Slice" or “Defocus” pull-down menu, EM images for all, or selected slices or defocus values will be displayed in sequence.

TIPS: If you choose "All" or “Select” both from "Slice" and "Defocus” pull-down menus, EM images for combinations of all, or selected slices and defocus values will be displayed in sequence.

TIPS: If you click “Image Tableau” check box, the selected images will be displayed in a table layout in terms of Slice numbers and Defocus values. In the example below, all the calculated images were displayed. You can specify the way of layout of slices and defocuses as well as gaps between each image in the dialog that will appear when you click “Tableau Setup” button (see Application section for more details).



TIPS: If you select “Atom Overlay” check box, a colored circle specific for each element will be drawn at each atom position as shown below. The size of the circle and its color will be modified with a dialog that will appear when you click “Setup" button.

NOTE: The gray-scale image can be printed out by using "Print" from "File" menu. The displayable gray levels depend on your printer specifications.

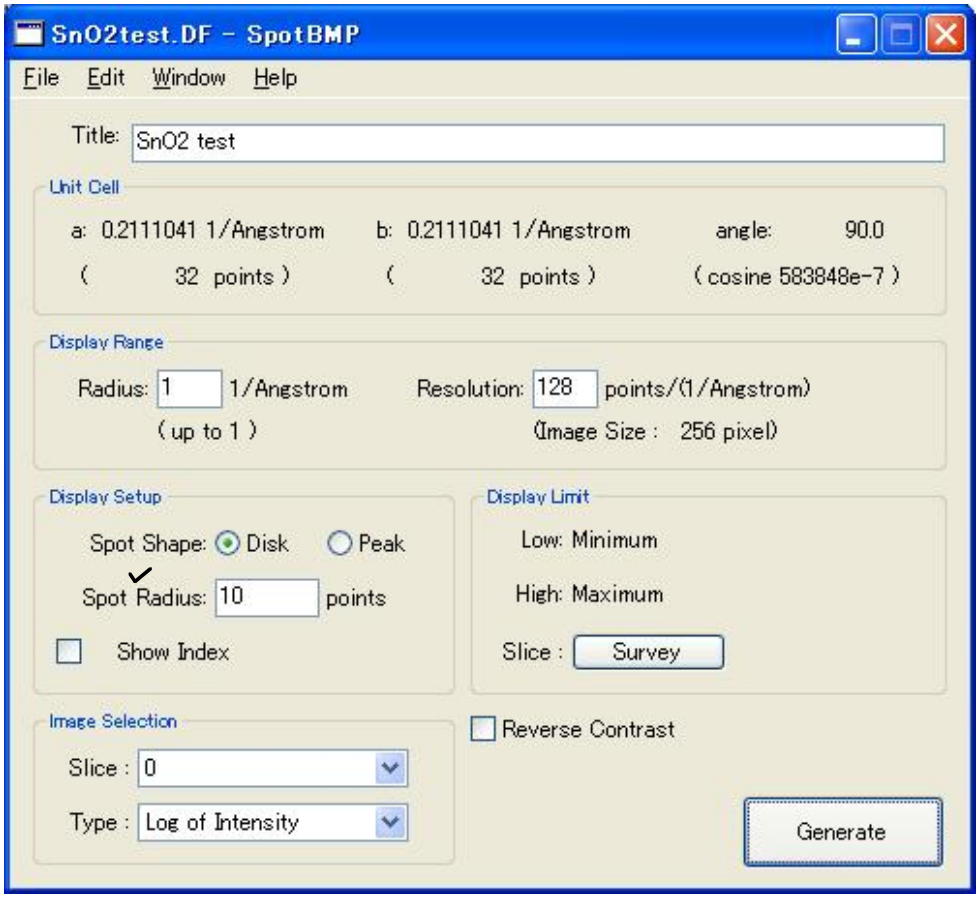
Diffraction Spot Pattern Display

Here, let's display electron diffraction patterns for SnO2 by using calculated scattering data with MultiGUI.

At first, you have to launch a utility and select a scattering data to be displayed:

1. Launch SpotBMP.
2. A data selection dialog will be opened. Select SnO2test.DF in the Data folder. (A data file for image display has ".DF".)

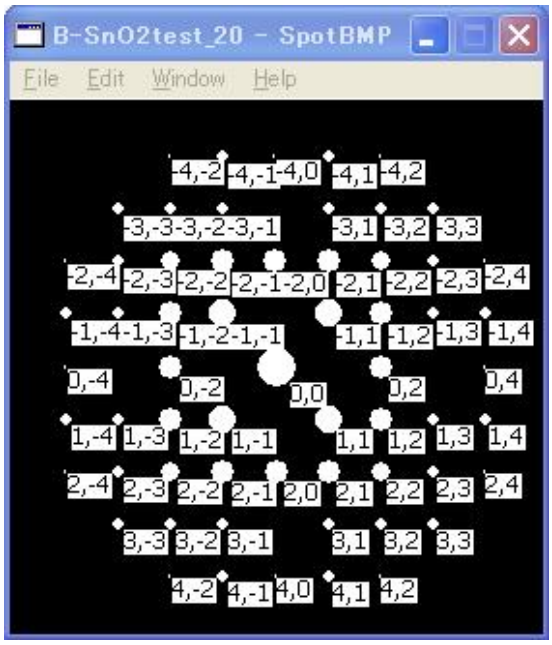
   A WORKSHEET for setting up display conditions will be appeared.



Then, let's get some diffraction patterns.

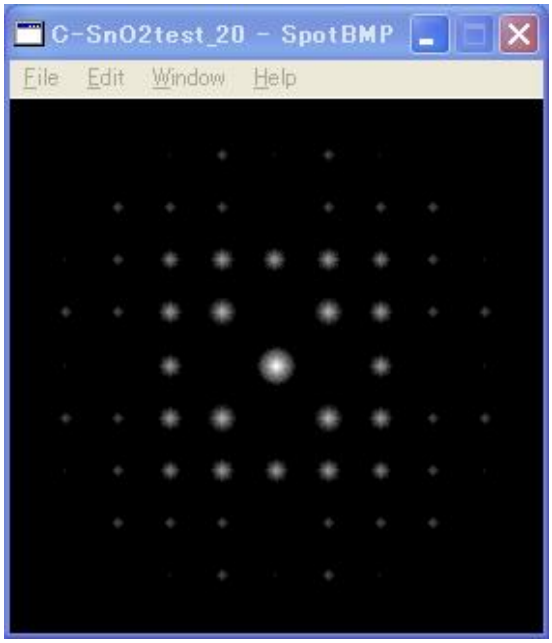
3. After setting the condition as shown above, click "Generate" in the right bottom of WORKSHEET.

   After a few seconds, you may get a gray-scale image shown below.



4. Next, uncheck the "Show Index" and select "Peak" from the "Spot Shape," then Click "Generate. "

   After a few seconds, you may get a gray-scale image shown below.



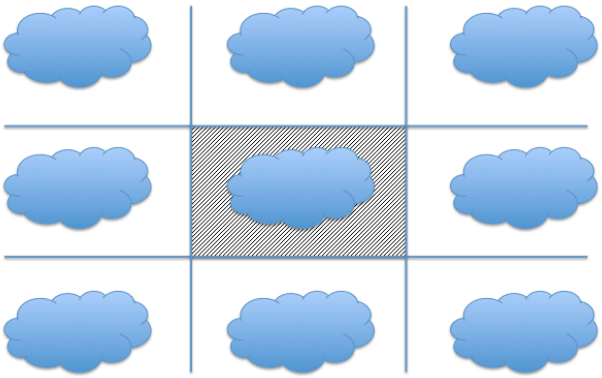
5. To terminate SpotBMP, select "Exit (Quit)" from "File" menu.

■ Topics

In this section some useful functions as well as advanced topics will be introduced. It is not necessary to read through all the topics at the first time. You may want to study each topic when you need to use it.

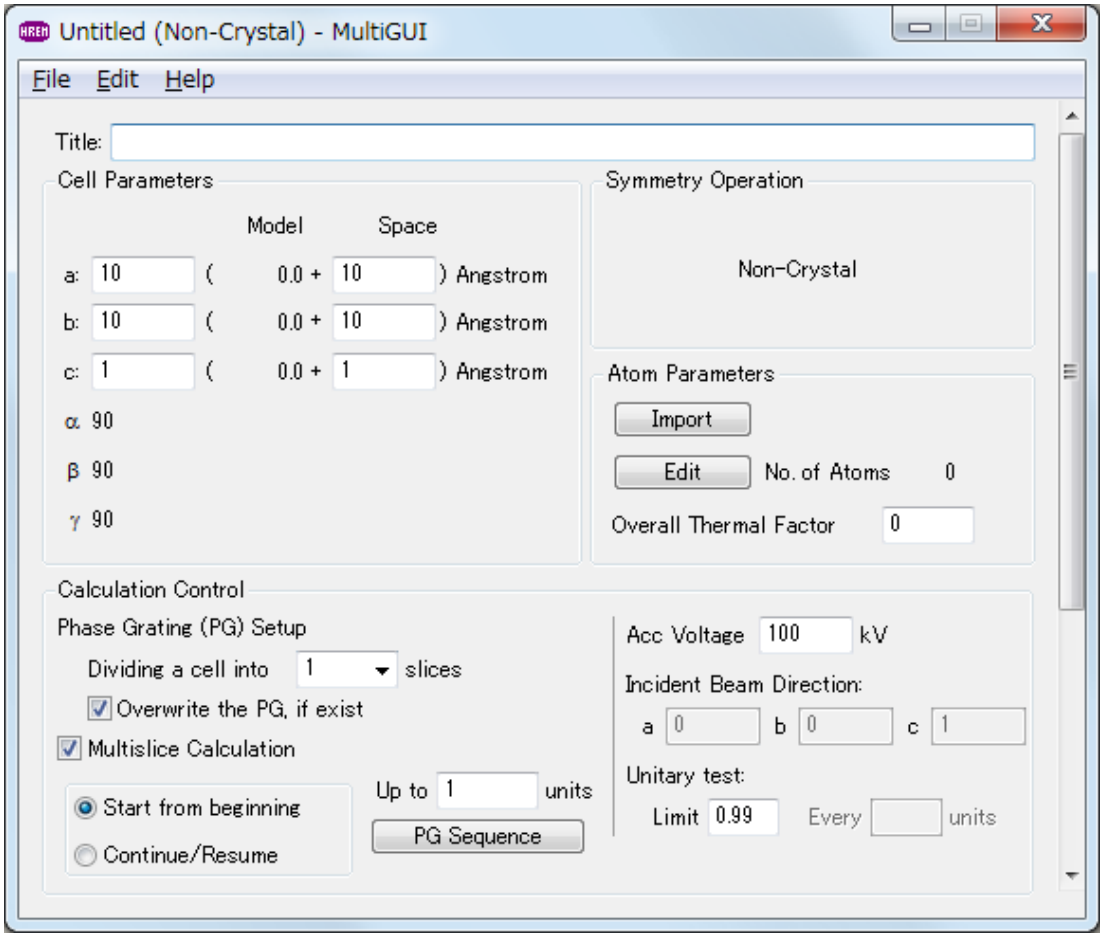
How to handle Non-periodic (Non-crystal) Model

xHREM intensively uses Fast Fourier transform that assumes a periodic continuation. Therefore, in order to simulate a model without a periodicity (non-periodic/non-crystal model), such as a nano-particle, we need a new device. xHREM handles non-periodic model using a big artificial cell (super-cell) that include the model. Here, a non-periodic model assumes that a super-cell is arranged as a 2D crystal as shown below.



The model size will be automatically calculated from the atom coordinates by the user interface. Furthermore, the model can be rotated to an arbitrary direction by using the xModelView, and then a simulation for that direction can be performed. In this case, the model size will be automatically calculated by the xModelView.

xHREM provides a graphical user interface shown below to make it easy to handle a non-periodic model.



The size of a super-cell can be defined by adding the Space to the Model size. Alternatively, the Space will be calculated from the super-cell size, if it is larger than the Model size. Here, the Space should be adjusted, so that any virtual neighboring models do not affect the results of simulation.

In the case of a non-periodic model, a space group or symmetry operations commonly used for a crystal model is not used. Furthermore, the lattice is restricted to an orthogonal system, and thus all the angles are always 90 degree.

If a non-periodic model is generated by using a super-cell, then the simulation can be performed in the same way as the crystal model. However, the size of a super-cell of a non-periodic model is usually larger than the unit cell of a crystal model. Furthermore, all the phase grating will be differ each other, and the number of the phase gratings becomes large, since there is no periodicity along the beam direction (z-direction).

Moreover, a calculation will be performed over only one super-cell (one unit) along the z-direction, since there is no periodicity along the z-direction of the non-periodic model. Thus, we can always use one (1) unit for the Up

to parameter, even if the super-cell is divided to any number of phase gratings, when you select Units for the Thickness in the Preferences.

Display Model Potentials or Wave-functions

Model potential distributions or wave-functions within the sample, which were calculated with MultiGUI (multi.exe), will be displayed as gray-level images by using ImageBMP.

To display them:

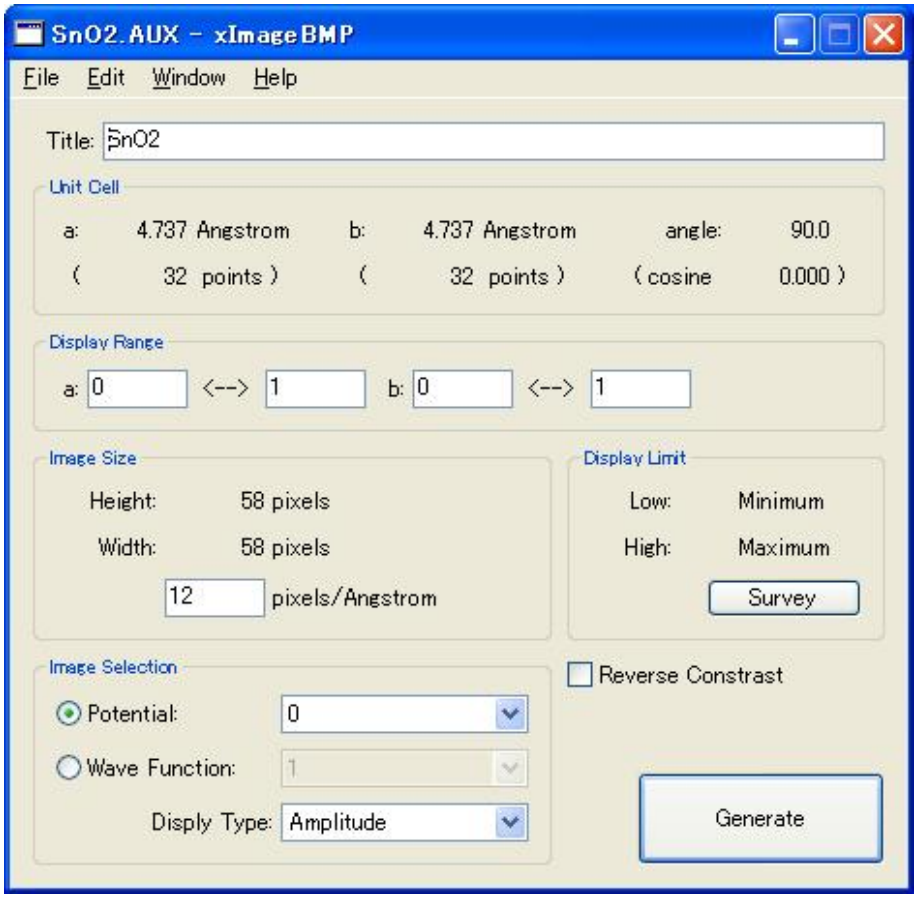
1. Execute a calculation with a check on corresponding "Export Data for Gray Scale Map" in the "Output Control" section of MultiGUI.

   The display data will be saved in a file with ".AUX" extension.

   NOTE: The file with the same extension is also used by ImageGUI to save microscope image data. Therefore, if you want to keep the data for later use, you have to change the AUX file name to a unique name keeping the same extension.

2. Launch ImageBMP, and select a corresponding AUX file.

   The following window, which you have seen for microscope image display, will be open. However, the "Image Selection" section is different from that for the microscope images, since the potential distributions and the wave-functions are saves as complex numbers.

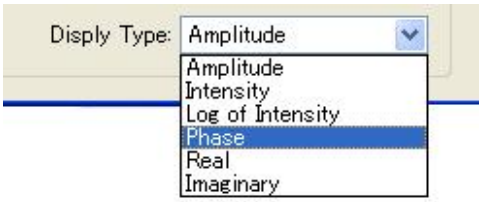


3. Setup display conditions and select what you want to display.

   Potential: You can specify a slice number (from 0 to 9) to be displayed, when you have divided a unit cell into different slices up to ten (10).

   Wave Function: Select a thickness (in slice number) to be displayed.

   Show: Since the potential distributions and the wave-functions are saves as complex numbers, you have to select a quantity to be displayed from the following list:



4. Click “Generate” to create a gray scale image.

Survey Diffraction Intensity

You can qualitatively compare dynamical diffraction intensities by looking a gray scale display generated by SpotBMP. When you want to compare the intensity quantitatively, you can use “DFOutGUI.”

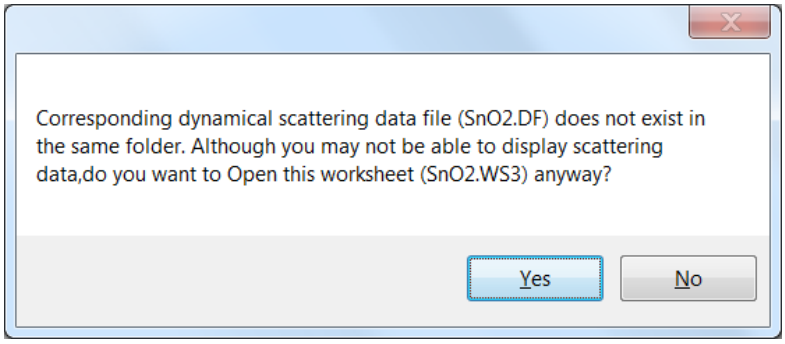
To survey diffraction intensities (amplitudes), you have to prepare the data as follows:

1. Launch DFOutGUI, and Choose “Open…” from File menu.

   NOTE: There is no WS3 file corresponding to the data name that we have used for the MultiGUI, namely SnO2test.WS3. We will create it from now using an existing data. You may create a WS3 data from a scratch by using Default.WS3.

2. Select SnO2.WS3 from the Data folder, when the open dialog appears.

   NOTE: When you haven’t finished dynamical scattering calculation for SnO2 data, you will get the following warning message. Then, press “OK” and continue the steps.

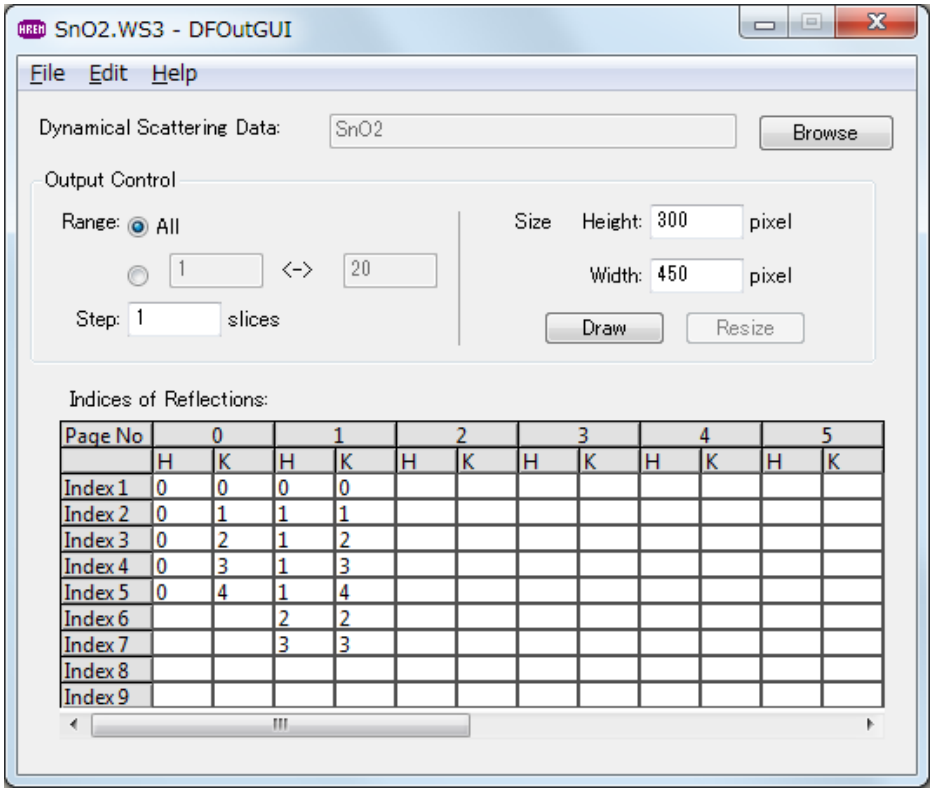

Corresponding dynamical scattering data file (SnO2.DF) does not exist in the same folder. Although you may not be able to display scattering data,do you want to Open this worksheet (SnO2.WS3) anyway?
Yes
No

   The WORKSHEET shown in the next page will appear.

   In this WORKSHEET, appropriate data is already filled out. Some reflection indexes are already specified for each page. Here, let's change Dynamical Scattering Data which has been calculated during the tutorial.

3. Open “SnO2test.DF” from “Browse” button, which is placed in upper right.
4. Choose "Save As..." from the File menu.
5. Save the new data as "SnO2test" in the save dialog appeared.

   TIPS: An extension '.WS3' will be added automatically. Thus, you may not need to specify the extension.

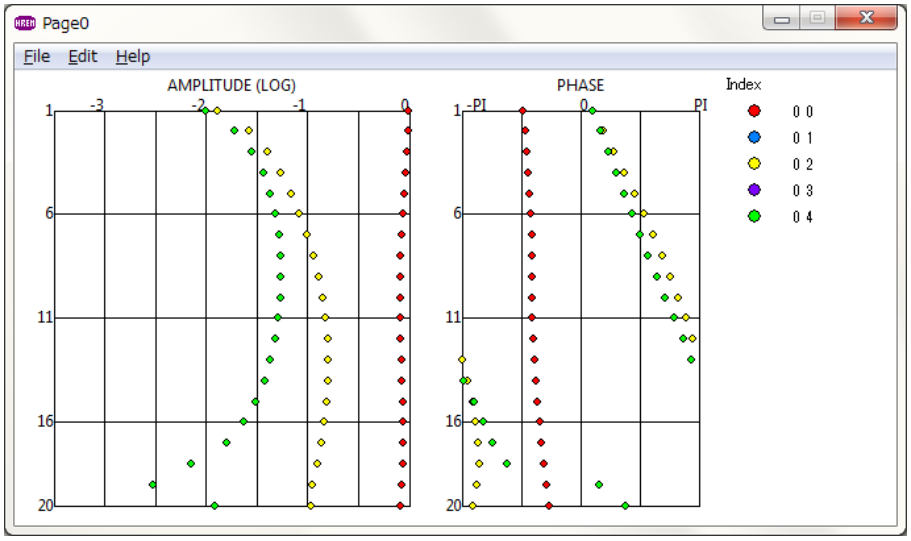


Next, we survey the image intensities by using the data saved above:

6. Click ”Draw” button.

   In the graphic chart the magnitude of amplitude is displayed in log scale to display a wide range of data. On the other hand the phase is displayed between [-π, +π]. You may note that this phase is shifted by π/2 to be consistent with the phase of kinematical structure factor.

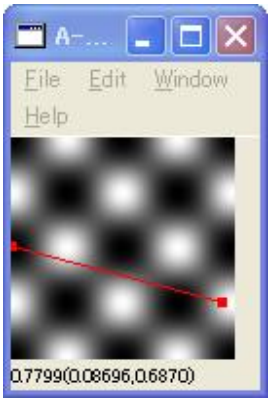
   You can change the width and/or height of the graph using “Resize”.



Survey image Intensity

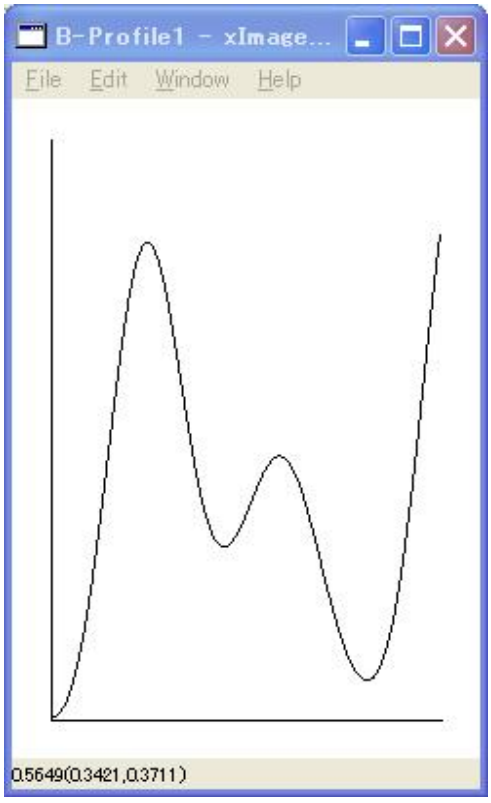
Electron micrograph images or wave-functions displayed by using ImageBMP will be surveyed quantitatively as explained below. Intensity profile along the specified line drawn on the image can be displayed and surveyed quantitatively.

Intensity on a gray scale image: When you move the mouse over a gray scale image created by ImageBMP, intensity under a mouse point is displayed at the lower part of window with its coordinates.



NOTE: An intensity value will not be displayed for an image created as an "Image Tableau."

Profile image: When you place a mouse on a starting point of a profile, and drag a mouse with SHIFT key down, a red line is drawn on the image. When you stop dragging, intensity under the red line is displayed on a separate window



When you put a mouse on a line of the profile window, intensity and its original image coordinates are displayed below the profile.

NOTE: A profile image will not be displayed for an image created as an “Image Tableau.”

3D Display of Atomic Model

Using a 3D display you can check your atomic model to be used by MultiGUI. Here, we explain the 3D display by using a sample data of SnO2.

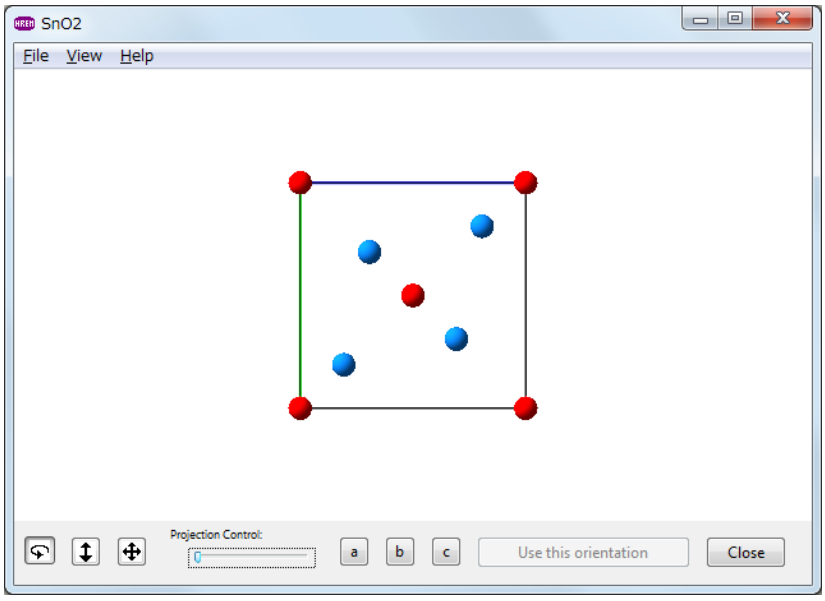
To display an atomic model as a 3D image:

1. Launch MultiGUI.
2. Choose "Open..." from the File menu to browse the sample data, and select “SnO2.WS1”.

   The WORKSHEET for SnO2 will appeare.
3. Click “Model View” in the Option section at the very bottom of the WORKSHEET.

TIPS: The lower part of the WORKSHEET can be accessed by sliding the window or by expanding the display area.

Then, you will get a 3D display of the Atomic model:

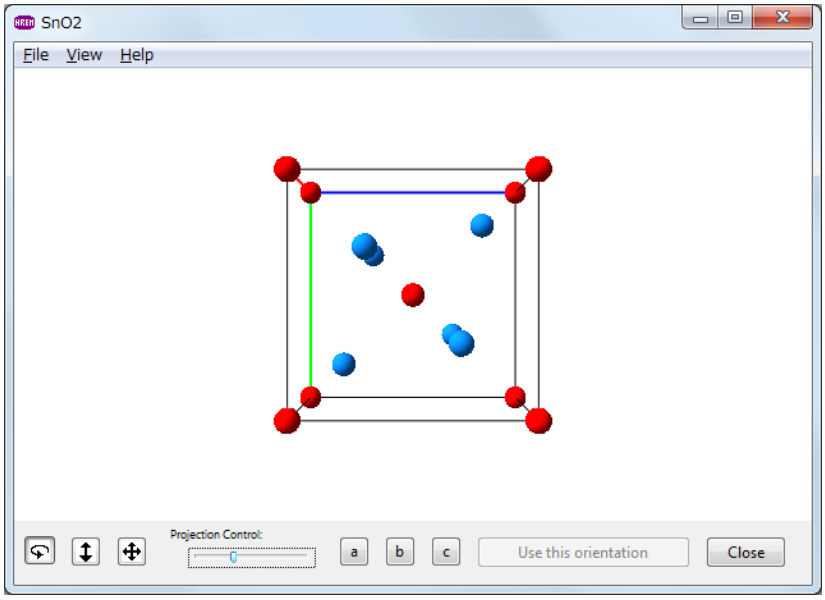


Under the regular setting the model is displayed as a projection along c-axis. The direction of projection is easily changed by selecting “a, b or c” in the tool bar.

TIPS: Tools in the tool bar (from left): Rotation, Back-and-forth movement, In-plane movement, Perspective control and Projection directions.

By adjusting a slider of the “Projection control” the model is displayed in

perspective drawing. The following show an example.

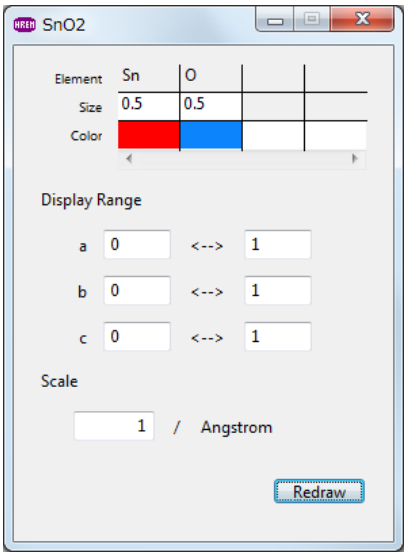


Use this orientation:

Crystal model: This button becomes active just after the orientation button "a, b, c" is pressed. If you close the xModelView by clicking Use this orientation, you can simulate the model at the selected orientation (the Crystal setting of the Preferences is changed accordingly).

Non-periodic model: You can simulate the model rotated to an arbitrary direction. After rotating the model to an arbitrary direction, close the xModelView by clicking Use this orientation.

TIPS: The size and color of each element, the range of the model to be displayed and the scale of display can be modified in the dialog that will appear when the View Options of the View menu is selected.

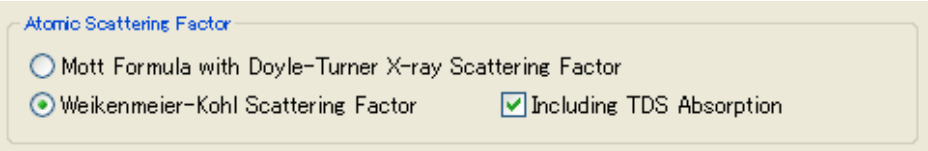


Including TDS Absorption

You can include absorption of elastically scattered wave due to thermal diffuse scattering (TDS) in your dynamical calculation. In this case, however, **thermal displacement parameter (temperature factor; Debye-Waller factor) for each atom in your atomic model is required**. When you don't know a corresponding parameter, an approximate value may be specified.

To include TDS absorption in your dynamical calculation:

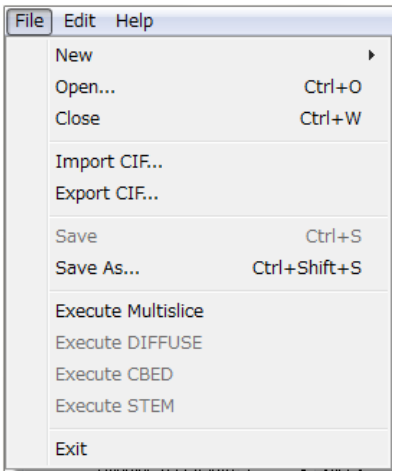
1. Launch MultiGUI
2. Choose "Preferences" from Edit menu.
3. Select "Weikenmeier-Kohl Scattering Factor" in "Atomic Scattering Factor" section of the Preferences dialog, and check "Include TDS absorption."


Atomic Scattering Factor
Mott Formula with Doyle-Turner X-ray Scattering Factor
Weikenmeier-Kohl Scattering Factor
Including TDS Absorption

4. Setup other parameters and execute "Multislice."

Data Sharing using CIF File

xHREM™ can read/write (Import/Export) a data with CIF (Crystallographic Information File) format. Therefore, you can share crystal data (lattice constants, Space group/Symmetry operations, Atomic positions etc.) with other software.



NOTE: The CIF data items handled by xHREM™: Lattice constants, Space group (Symmetry operations), Atom species, Atom coordinates, Thermal factor, Occupancy.

xHREM for Windows and Mac OS stores atomic model data such as atomic positions with the same database format. Therefore, the atomic model database can be freely shared between Windows and Mac OS.

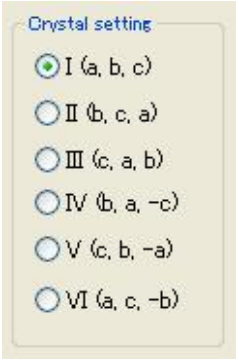
NOTE: You can also share an atomic model data with other applications by saving them as a text file using "Export" button on the "Edit" window of "Atom Parameters" section of MultiGUI.

Permutation of Crystal Axes

xHREM™ can take account of an incident surface effect into dynamical calculation (K. Ishizuka: Multislice Formula for Inclined Illumination: Acta Cryst. A38 (1982) 773-779). Therefore, an incident beam direction of <hk0> that is parallel to the surface is forbidden.

However, when you neglect the incident surface effect (most of the programs do not take into account the surface effect), you can straightforwardly calculate for <hk0> incidence by using a capability of permutation of crystal axes without changing a model data.

To permute the crystal axes, choose "Preferences" from Edit menu of MultiGUI. Then, you may notice "Crystal Setting" on the upper right of the Preferences window as shown below:



For example, in the case of <110> incidence we cannot use I (a.b.c) system, since the index of the third axis (c-axis) is zero. However, indexes of both a-axis and b-axis are not zero, and thus we can use either these axes for the third axis. Therefore, we can choose one system from II, III, V or VI for the <110> incidence. Contrary to this, in the case of <100> both indexes of b- and c-axes are zero, and thus we cannot use both of them as the third axis. Therefore, we can use either II or V system where a-axis is the third axis.

NOTE: Neither the crystal axes nor symmetry operations are permuted in the WORKSHEET of MultiGUI. Nevertheless, the selected crystal system is used in calculation, and symmetry operations are transformed accordingly. When you check the list output, you can verify the lattice constants, atom parameters, and symmetry operations actually used in calculation.

Calculation of Static Diffuse Scattering

Since xHREM™ can handle up to 1,000,000 atoms, diffuse scattering due to static disorder of atom positions can be estimated by using an atomic model including static displacements of atom positions.

To calculate diffuse scattering due to static disorder:

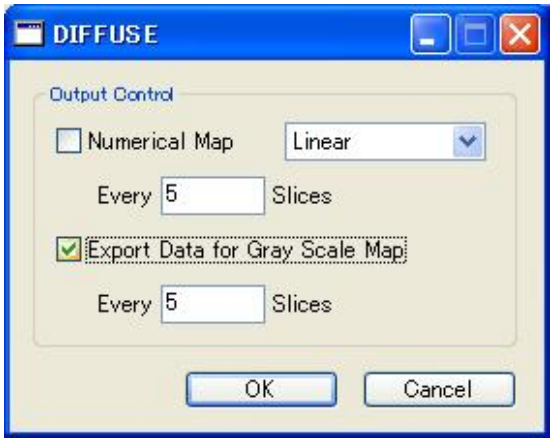
1. Launch `MultiGUI`.
2. Input necessary data in the WORKSHEET as usual.

   Using "Edit" dialog of "Atom Parameters" of MultiGUI, it may be difficult to prepare a large atomic model including static displacements of atom positions. Therefore, it may be convenient to read a text data file of atomic model created separately by using "Import" capability.

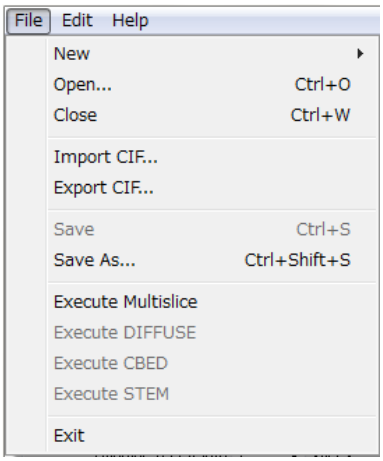
3. Click "DIFFUSE" in the Option section at the very bottom of the WORKSHEET.

TIPS: The lower part of the WORKSHEET can be accessed by sliding the window or by expanding the display area.

The following dialog will appear, where you can specify some output controls specific to DIFFUSE calculation. Change controls as you want, and Click "OK."



4. Save your data.
5. Choose "Execute DIFFUSE" from File menu.



The program (diffuse.exe) that calculates the diffuse scattering amplitudes will be launched, and the progress of calculation will be displayed on a separate window. When an execution terminates normally, you will see the message "Execution completed. Congratulations!"

NOTE: The progress window has the fundamental menus such as File and Edit, and you can Save the content of the window from the File menu.

TIPS: The program can be terminated even in the middle of calculation by Exit command from the File menu or clicking the close button.

The progress window can be closed by Exit command from the File menu or clicking the close.

6. To terminate MultiGUI, select "Exit (Quit)" from "File" menu.

Display Diffuse Scattering Distribution

"ImageBMP" can be used to display diffuse scattering distributions. Diffuse scattering data is saved in a file with ".ED" extension.

To display diffuse scattering patterns:

1. Launch ImageBMP.
2. Open a ".ED" file with an appropriate name.
3. Setup display controls.

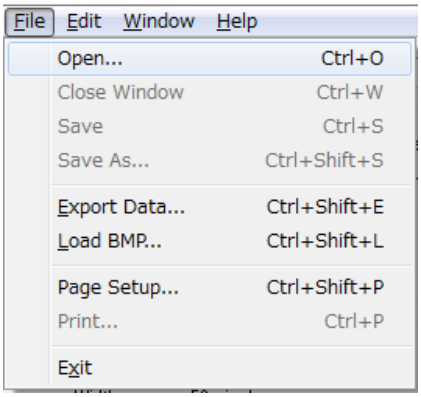
   According to "ImageBMP" instructions setup an image display area, the resolution and so on, and select a thickness in slice number to display scattering pattern.

   Since a scattering data is save as complex numbers, a data type to be displayed will be selected from "Show" list.
4. Click "Generate" to display a gray scale map.

Numerical Data Output Using ImageBMP

"ImageBMP" displays a gray scale image of various data as a Bitmap. A numerical value of each pixel of the gray scale map can be output for further analysis with other application, such as Gatan's DigitalMicrograph. A numerical data used to generate the gray scale map can also so be output.

The file menu of ImageBMP and the image display windows have "Export Data…" command as shown below:



A numerical data used to generate the gray scale map can be output using the "Export Data…" command of ImageBMP.

A numerical value of each pixel of the gray scale map can be output using the "Export Data…" command of each image display window.

Output format for numerical data:

The following data format(s) will appear in the "Save as type" list in the Save As dialog.

Real data	TIFF output (.tif) Binary output (.pfm: Portable Floatmap File) Text output (.csv: Comma Separated Values File) Gatan format (.gfx)
Complex data	TIFF output (.tif) Binary output(.pcm: Portable Complexmap File) Gatan format (.gfx)

Output format for numerical data:

Real data	TIFF output (.tif) Binary output (.pfm: Portable Floatmap File) Text output (.csv: Comma Separated Values File) Gatan format (.gfx)

NOTE Portable Floatmap/Complexmap File (.pfm/.pcm) format has a text header. xHREM uses a header of 192 bytes including an image size.

Application

In this chapter
we explain how to create your own data,
and the way to customize xHREM™
by using Preferences and Templates.
Then, you will see a detailed explanation for each data item
of the Graphical User Interfaces.

■ Let's attack a problem in hand

Before proceed to this chapter, please get acquaintance with xHREM by going through the examples of the "Getting Started." In this chapter, you will learn how to create a new data for your own problem, and then how to display your results and more…

Steps to create a New Data

There are two ways to create a new data for your application:

- Update an existing data
- Create a data from scratch

To create a new data from an existing data, do this:

1. Launch a corresponding graphical user interface (GUI).
2. Choose “Open…” from File menu, and select an existing data you want to copy in the file selection dialog.

   The WORKSHEET will appear with data you select.
3. Save this data with a new name by choosing "Save As…" from File menu.

NOTE This step is strongly recommended not to lose the existing data by an accidental overwrite.

4. Then, change data as you want.
5. When finished, save your modified again data by choosing "Save" from File menu.

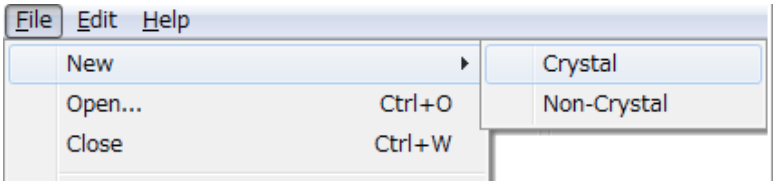
If you want to use another existing data, select it using Open... command.

To create a new data from a scratch, do this:

1. Launch a corresponding graphical user interface (GUI).
2. The Default (blank) work sheet for a crystal data will be opened. If you want make a non-Crystal data, then choose “Non-Crystal” from “New” command of File menu.

   The WORKSHEET named "Default (Crystal)" or "Default_NonCrystal (Non-Crystal)" will appear with some default data.
3. Fill out your data in the WORKSHEET.
4. When finished, save your data with a new name by choosing "Save As…" from File menu.

If you want to use another new data, select “Crystal” or “Non-Crystal” using New command.



The WORKSHEET named "Default (Crystal)" or "Default_NonCrystal (Non-Crystal)" will appear with some default data.

Setting up Preferences

The Preferences hold some control data that does not depend on each sample.

The calculation programs (Solvers) only accept the data with a definite format and units. However, you may want to use other units in your WORKSHEET. You can choose your preferred units for your input in "Preferences" window.

To set up the Preferences:

1. Choose "Preferences" from "Edit" menu of MultiGUI or ImageGUI.

The following "Preferences" window will open.

TIPS: The first choice of Units or Defocus sign is used in the calculation program. The data specified in other units will be converted by the graphical user interface (GUI).

2. Change settings according to your preference.

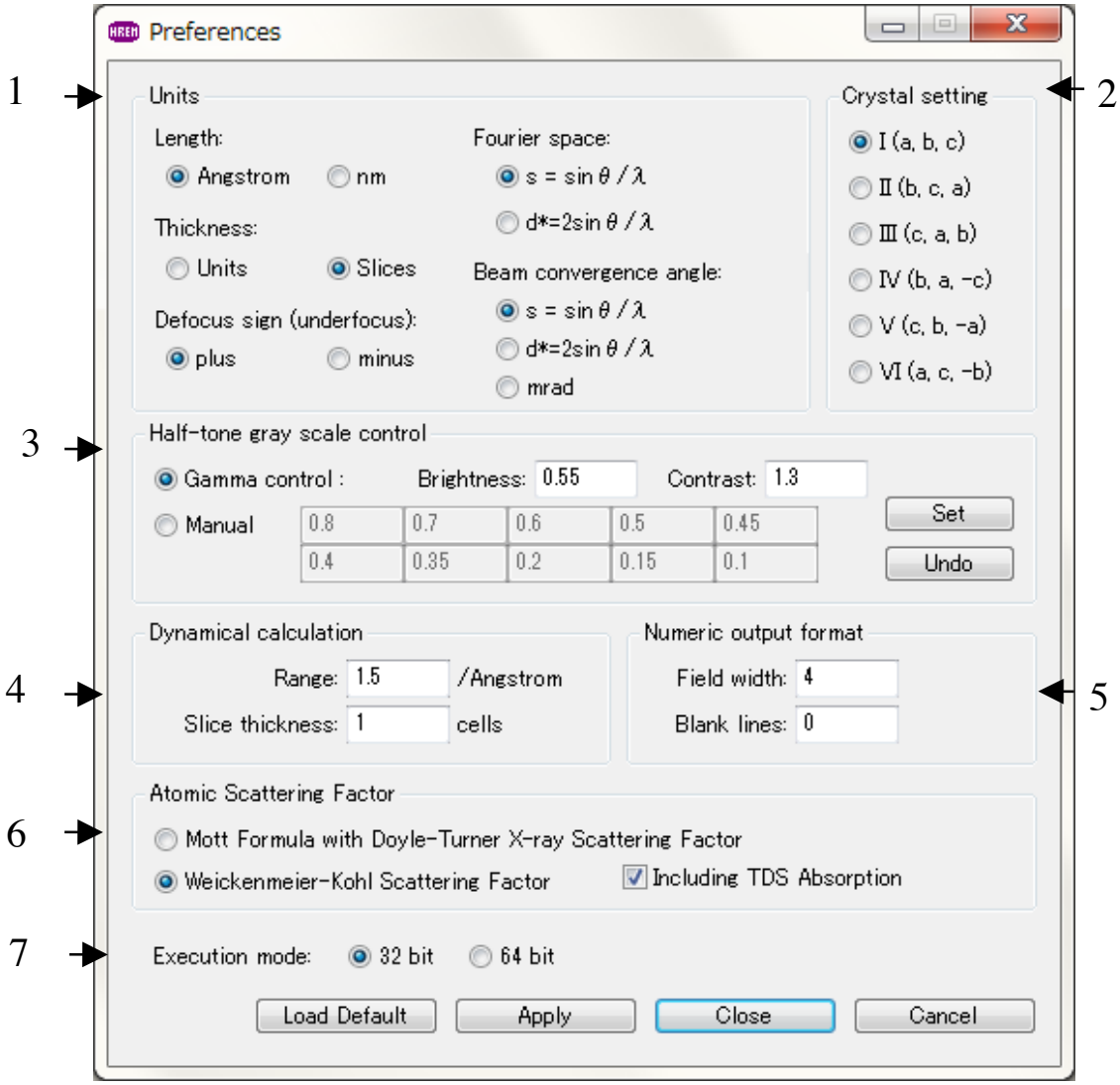
   "Apply" will change the WORKSHEET according to the change(s).
3. Click "Close" or “Cancel” to close the Preferences window.

   When “Close” is clicked, the current settings of the Preferences will be applied on the WORKSHEET.

When "Cancel" is clicked, the settings after the last “Apply” will be discarded. (These changes have no influence on the WORKSHEET.)

NOTE: You cannot restore the change(s) already applied to the WORKSHEET by clicking “Cancel.” In order to restore the change(s) on the WORKSHEET, reset the Preferences and press "Apply."

TIPS: We recommend you to verify your change(s) on the WORKSHEET by clicking "Apply" before closing the Preferences window by clicking "Close."



The first choice of Units or Defocus sign is used in the calculation program. The data specified in other units will be converted by the graphical user interface (GUI).

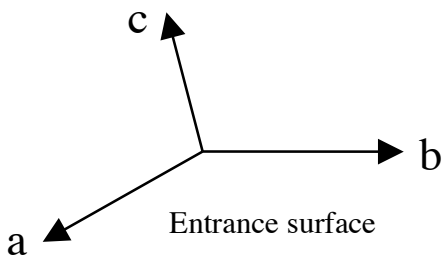
1. Units
   Length: Angstrom, nm

Thickness: Unit cells or slices
Defocus sign (underfocus): plus, minus
Fourier space: s, d*
Beam convergence angle: s, d*, mrad

TIPS: Calculation programs use the unit that is the first in the selection list. Therefore, the Graphical User Interface (GUI) converts the value specified in other unit to the standard unit necessary for a calculation.

2. Crystal setting

   I (a, b, c)



   II… Axes are permutated as indicated

3. Half-tone output settings

   Level settings for character-base half-tone output (11 levels)

4. Dynamical calculation

   Range: Radius of Fourier space to be included in the calculation
   Slice thickness (cell numbers): to be used for the projection approximation

5. Numerical data output format

   Field width: Number of characters including blank(s)
   Blank lines: number of line feed(s)

6. Atomic Scattering Factor

   When you want to include TDS absorption using Weickenmeier-Kohl scattering factor, you have to specify a thermal factor (Debye-Waller factor) for each atom as an atom parameter.

   Doyle-Turner scattering factor can be used up to only s=2.0 (d*=4.0) due to its approximation.

7. Execution Mode

   Select the execution mode from a 32bit or 64bit according to your license.

   Note: The 64bit module becomes available from v3.9. Therefore, there is a fee-charging upgrade path from a 32bit module to a 64bit module.

Creating Your Template WORKSHEET

Graphical user interface (GUI) uses a WORKSHEET for data preparation. xHREM is shipped with WORKSHEETs (Default.WS1 etc.), on which some standard values are already specified. We call these WORKSHEETs

having standard values as "Default (Template)." When you create a new data, you can save your trouble to input these common data at each time by using the Default WORKSHEET.

Moreover, you can prepare the data with less effort by using the WORKSHEET tailored for your experimental conditions. For examples, an acceleration voltage, an output range for dynamical scattering amplitudes etc. for the scattering calculation, or a spherical aberration coefficient, a defocus spread, a bean convergence angle, an aperture radius etc. for the image intensity calculation. You can create a template WORKSHEET with other preferential settings.

Creating a template WORKSHEET will follow the same steps as preparing the new data. However, only default data items are specified instead of filling out all entries.

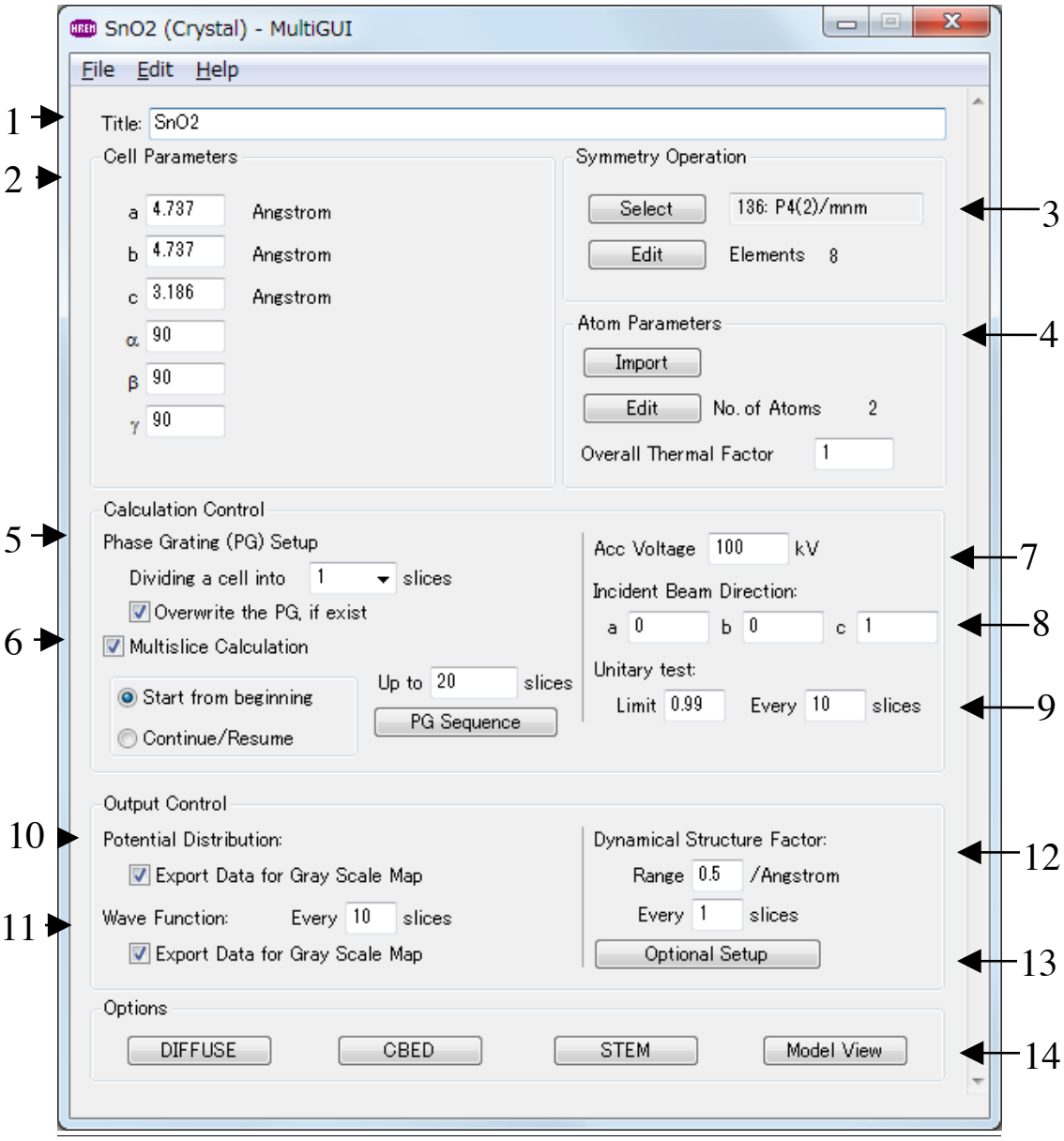
To create a new data from a scratch, do this:

1. Launch a graphical user interface (GUI) for which you want to create a template.
2. Select "Default" from the file selection dialog.
3. Specify default data items.
4. Save your WORKSHEET with a specific name, which reminds you that it is a template data.

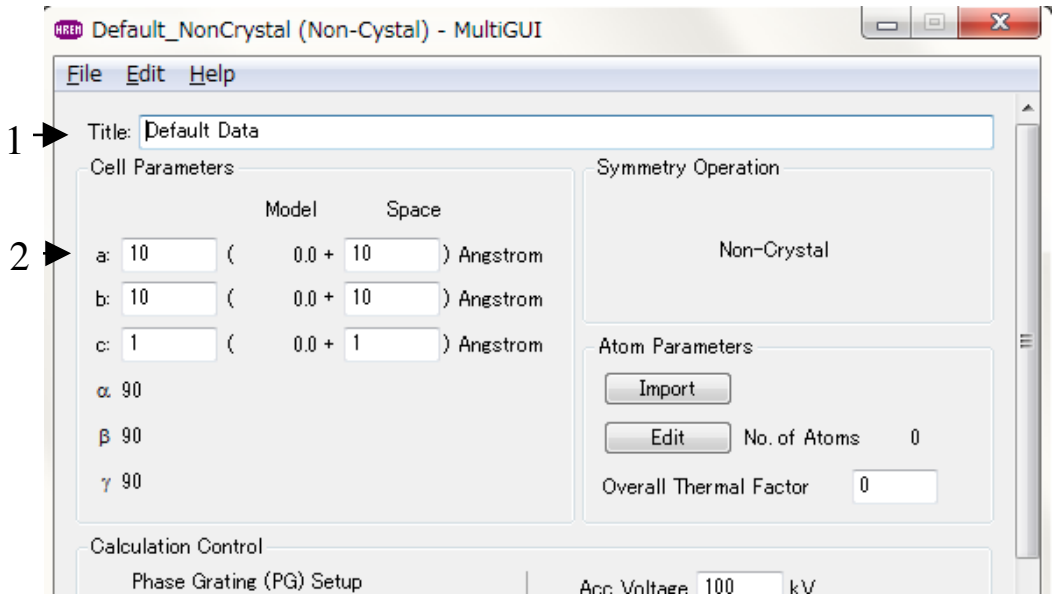
   From next time, you can start with your template saved above and save your trouble by using these predefined data items.

■ MultiGUI Reference

WORKSHEET (Crystal)



WORKSHEET (Non-Crystal)



1. Title (max. 82 characters)

   Type a sample name, composition, and experimental conditions etc. as you want.

2. Cell Parameters

   Specify cell lengths and angles. The cell lengths can be given Angstrom or nm according to your preference. The angles can be given in degree or cosine of the angle. A mixed input of angle in degree or cosine is not allowed. (Input in angle is recommended.)

   In the case of a non-periodic/non-crystal model the size of the super-cell that is the sum of a model size and a space (vacuum).

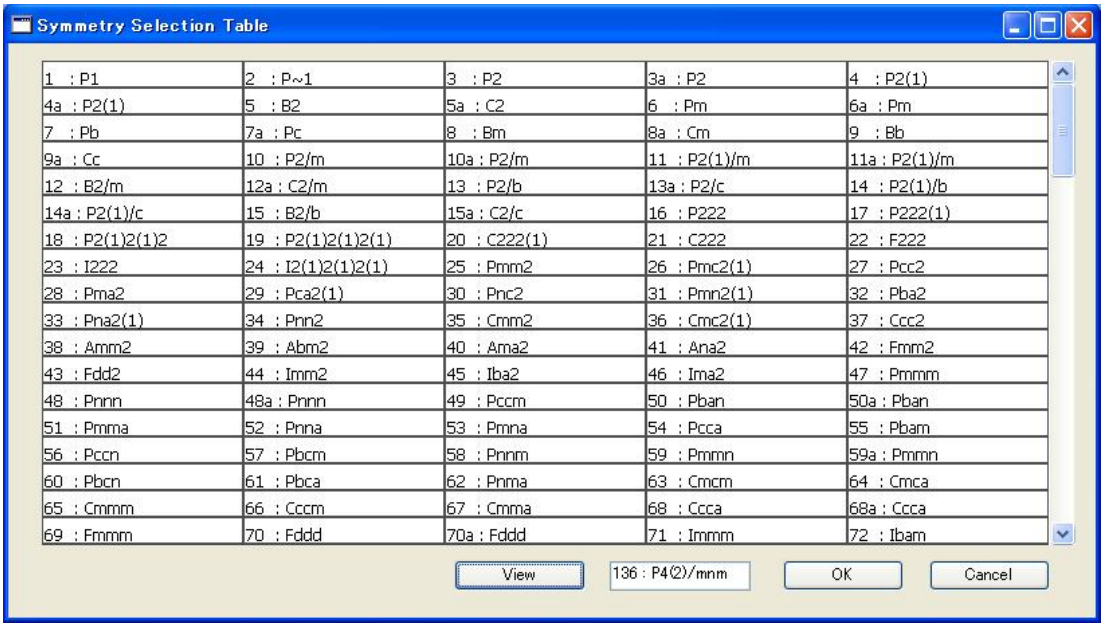
3. Symmetry Operation

   You can specify symmetry operations by selection one of the space groups by clicking "Select" or edit them by clicking "Edit."

   Note: In the case of Non-Crystal the space group cannot be select. The space group P1 is always assumed.

"Select" button:

Clicking the "Select" button will open the following window showing all possible space groups. Select one of the space groups corresponding to your specimen. The space group you have selected will appear in the box.

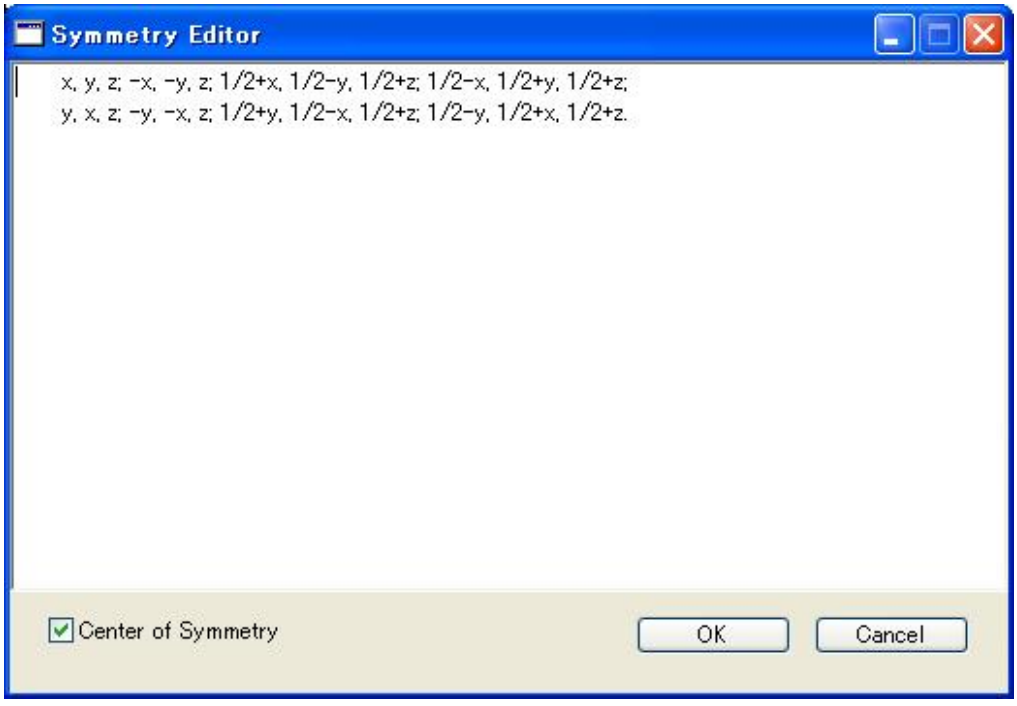


You can see symmetry elements in the window (see "Edit" button below) appeared by clicking the "View" button. Please confirm the symmetry elements are correct before proceeding the calculation.

"Elements": Number of symmetry elements

"Edit" button:

Clicking the "Edit" button opens a window where you can specify arbitrary symmetry operations.



Symmetry operations should be specified according to the conventions used in International Tables for Crystallography.

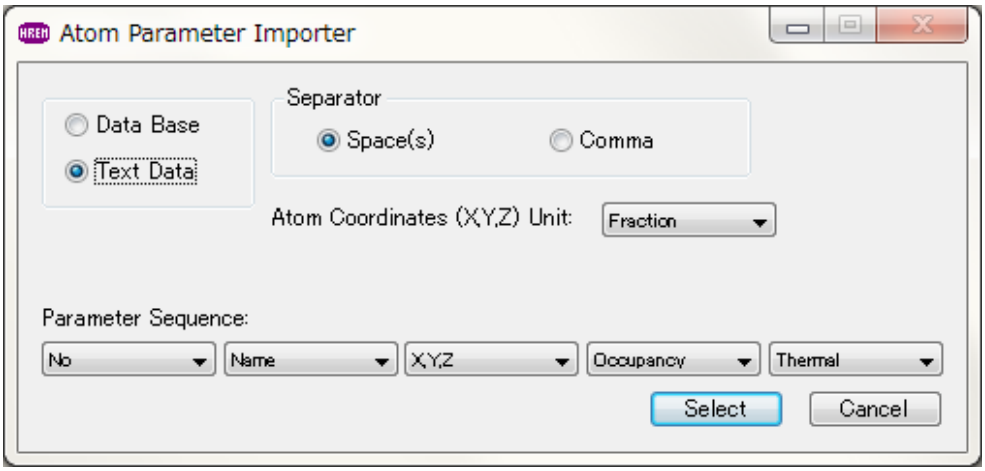
- xyz components of each symmetry operation should be separated by a comma (,)
- Each symmetry element should be separated by a semicolon (;)
- Symmetry list should end with a period (.)

4. Atom Parameters

Atom parameters will be imported from a data file by choosing "Import" or compiled in the window that will appear by choosing "Edit."

"Import" button:

Clicking the "Import" button will open the window to select an existing atom parameter file.



- Data Base: atom parameters already saved by MultiGUI.
- Text Data: atom parameters saved in the text format.
  Data Separator: space(s) or comma can be used as a data separator
  Parameter Sequence: the order of data items will be specified. If there is no corresponding data item in the file, you may use "None" to skip reading it.

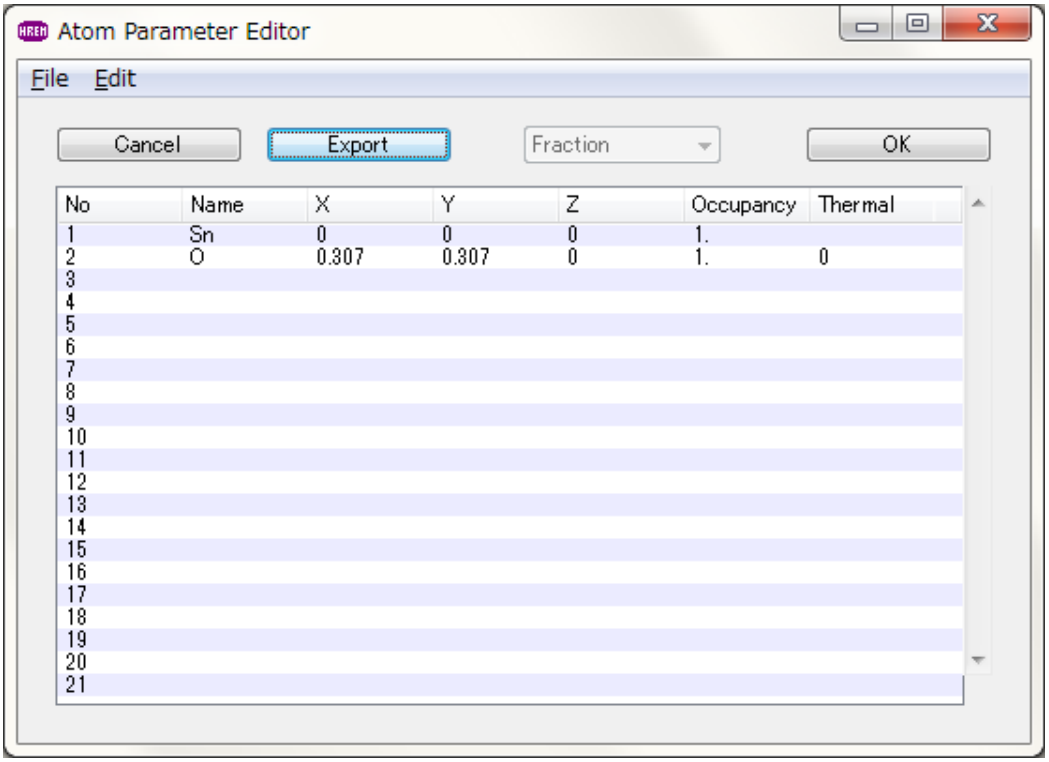
Data file will be selected in the dialog that appears by clicking the "Select" button.

Input unit of atom coordinates: Unit of the atom coordinates can be selected using Atom Coordinates Unit pull-down.

When the atom parameters are imported successfully, these parameters will be displayed in the window (see "Edit" button below).

"Edit" button:

Clicking the "Edit" button opens a window where you can compile atom parameters on the spot.



- No: sequence number added automatically
- Name: atom name including element name. Ex. Ag, C(1), O-2
- x, y, z: atom position in the unit cell defined by a fraction
- Occupancy: ratio of occurrence of atom (normally, one). This parameter may be omitted.
- Thermal: isotropic thermal displacement factor. If you input zero (or leave blank), then the Overall Thermal Factor (see the next parameter) will be applied in the calculation.

Export: Atom coordinate data is exported as a text format data (fixed data length), whose extension is. atm.

Atom coordinate unit: When creating a non-crystal manually, an atom coordinate unit is selected from Angstrom/nm.

No of Atoms: number of input atoms

Overall Thermal Factor:

Isotropic thermal displacement factor that will be applied for each atom in the crystal. If the thermal displacement factor of each atom is specified as zero or left blank, this thermal displacement will be used for that atom in the calculation.

Calculation Control

5. Phase Grating Setup

   Dividing-a-cell-into box: Select a number of divisions of unit cell (up to thousand (1000)). The phase grating number up to 10 can be selected from the pull-down list. If you want to use more than 10 phase gratings, simply input a number (up to 1000) of phase gratings t.

   ☐ On/off Overwrite the PG, if exist

   The phase gratings (PGs) will be calculated automatically, if necessary. This check box controls whether a new PGs are calculated, or the existing PGs are used, when the PG file of the same name is exist.

6. Multislice Calculation

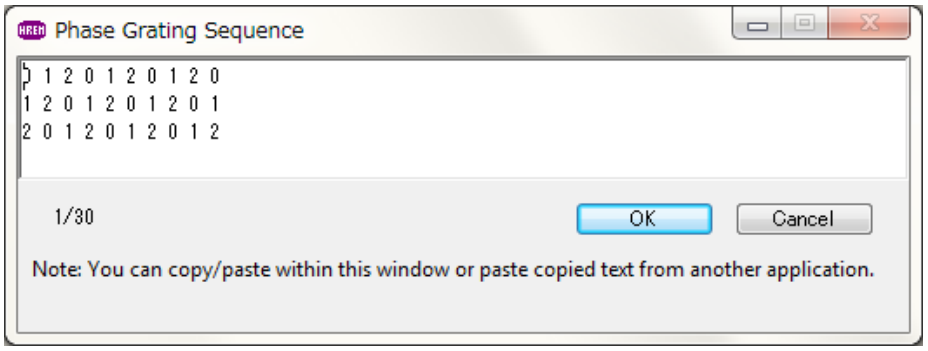
   ☐ On/off multislice calculation

   Up to box: set the last sample thickness in unit cell of slice number (up to 9,999 slices)

   Start from beginning & Continue/Resume buttons: select "Start from beginning" when you start a new calculation, or "Continue/Resume" when you continue calculation by increasing the last sample thickness. In the case of STEM calculation, if you stopped the calculation in the middle, you can resume calculation from the next scan point using "Continue/Resume".

   NOTE: In the case of STEM calculation you cannot continue calculation by increasing the last sample thickness.

   PG Sequence buttons: A default phase grating sequence is a cyclic repetition of 0 to the number of phase grating. You can edit the sequence using the Sequence Editor that appears by clocking the “PG Sequence” button.


Phase Grating Sequence
0 1 2 0 1 2 0 1 2 0
1 2 0 1 2 0 1 2 0 1
2 0 1 2 0 1 2 0 1 2
1/30
OK
Cancel
Note: You can copy/paste within this window or paste copied text from another application.

   The sequence is specified by the space-separated phase grating numbers.

7. Acc. Voltage
8. Incident Beam Direction

   Specify an incident beam direction in term of a real lattice coordinates. Ex: [001] incidence.

9. Unitary Test: A test for the sum of scattering intensity

Limit: A number close to one imposes a strict condition.

Cycle: Frequency for the test in the sample thickness unit

Output Control

10. Potential Distribution
    - ☐ On/off file output for gray scale display

11. Wave Function
    - ☐ On/off file output for gray scale display

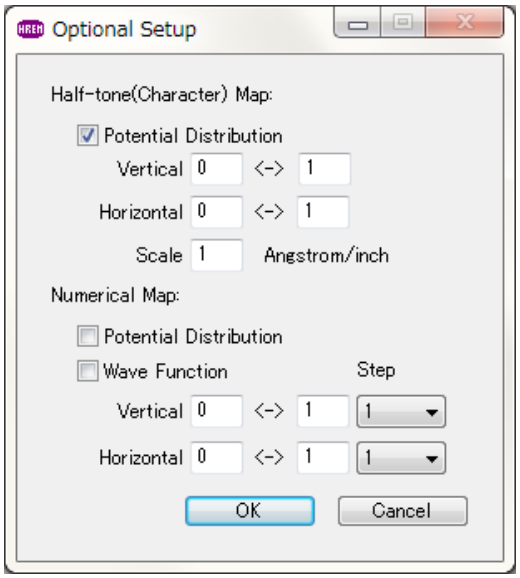
    Cycle: Frequency for the file output in the sample thickness

12. Dynamical Structure Factor

    Range: File output range (radius) of scattering amplitudes

    Cycle: Frequency for the file output in the sample thickness

13. Optional Setup



Half-tine Map

- ☐ On/off Potential distribution

Vertical and horizontal ranges and scale for half-tone output

Numerical Map

- ☐ On/off Potential distribution
- ☐ On/off Wave-function

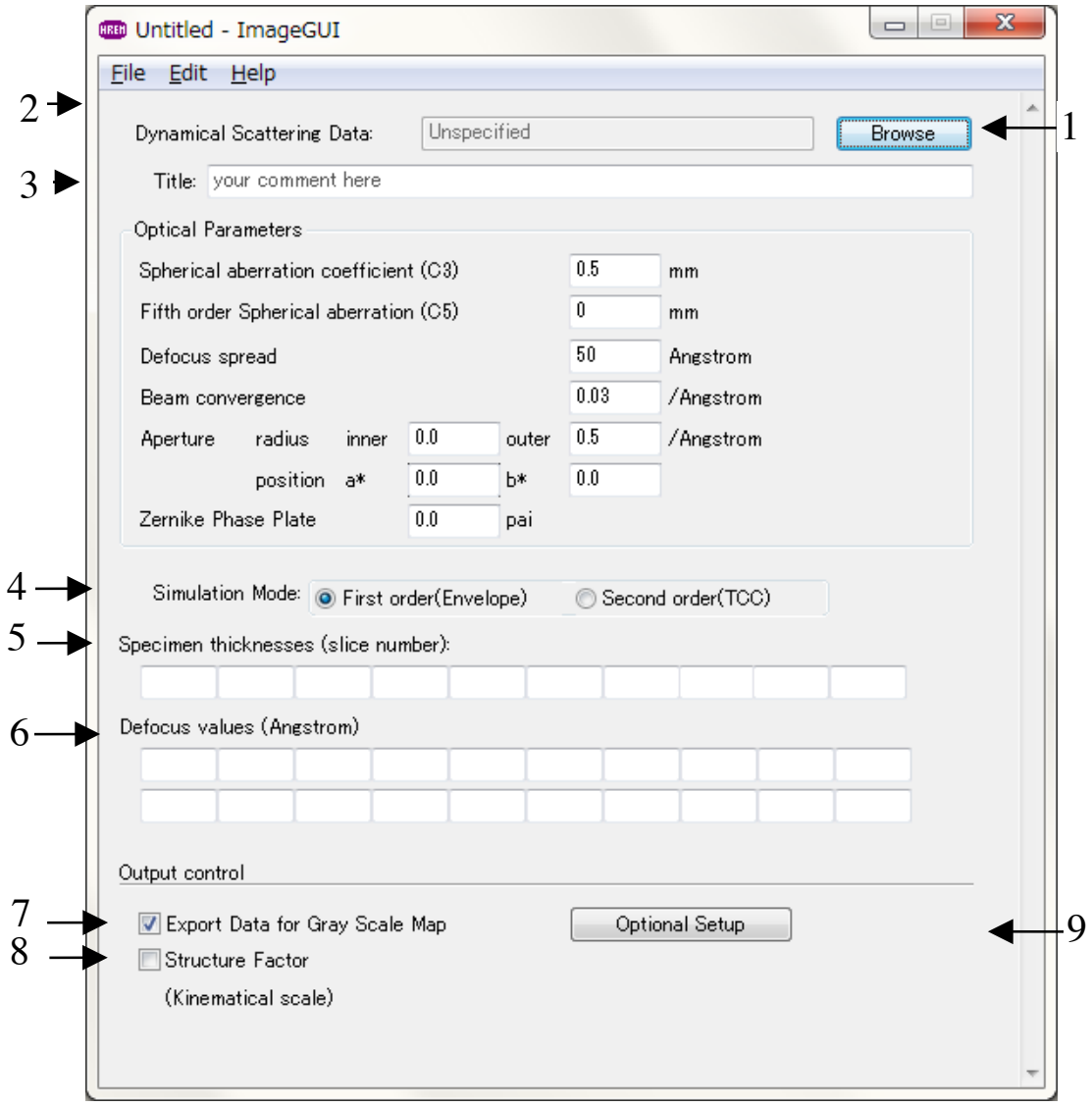
Vertical and horizontal ranges and steps for numerical map output

Options

14. Additional function setup dialogs and xModelView

    CBED and STEM are extensions to xHREM, and require additional licenses.

WORKSHEET



1. Dynamical Scattering Data
   Select the scattering data that is calculated with MultiGUI using the Browse button.
2. Title (max. 82 characters)

   Type a sample name, composition, and experimental conditions etc. as you want.
3. Optical Parameters
   - Spherical aberration coefficient (C3)
   - Fifth order Spherical aberration (C5)

- Defocus spread
- Beam convergence
- Aperture radius: inner and outer positions
- Zernike Phase Plate

  Specified phase shift will be applied in the area inside of the inner aperture. If the phase shift is zero, the beam within the inner aperture is blocked.

4. Simulation Mode

   Partial coherency will be treated by First order (Envelope) approximation or Second order (TCC) approximation.

5. Slice thicknesses

   Specimen thickness at which EM images will be calculated will be given in terms of slice number (up to 10 slices).

6. Defocus values

   Defocus values at which EM images will be calculated will be specified (up to 20 values). Sign and unit of defocus will be changed by Preferences settings.

Output Control

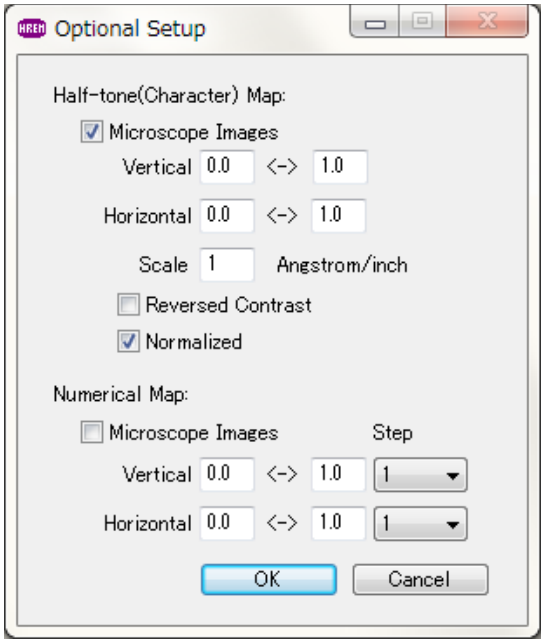
7. Export Data for Gray Scale Maps (Microscope Images)

   If you select this option, binary data will be exported to the file for later fray scale display using Image BMP.

8. Structure Factor

   If you select this option, structure factors will be listed before image calculations for each lice data.

9. Optional Setup



Half-tone Map

- ☐ On/off Microscope Images

Vertical and horizontal ranges and scale for half-tone output

- ☐ On/off contrast reversal
- ☐ On/Off normalization

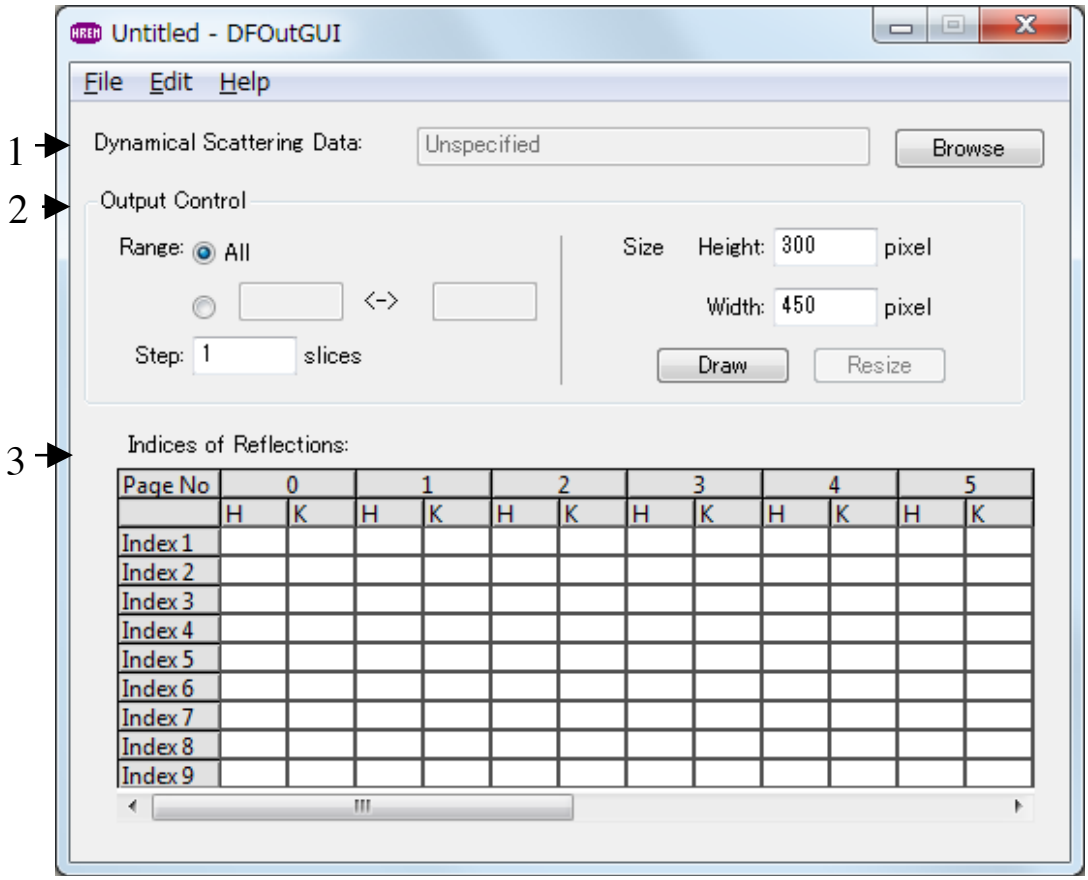
Numerical Map

- ☐ On/off Microscope Images

Vertical and horizontal ranges and steps for numerical map output

■ DFOutGUI Reference

WORKSHEET



1. Dynamical Scattering Data
   Select the scattering data that is calculated with MultiGUI using the Browse button.
2. Output Control

   Output Range: Thickness for a list and/or graph output will be specified by its range and step in slice unit.

   Size: Specify the size of graphical output window.

   Draw: Draw graphical output.

   Resize: All graphical output will be redrawn with the specified window size.
3. Indices of Reflections

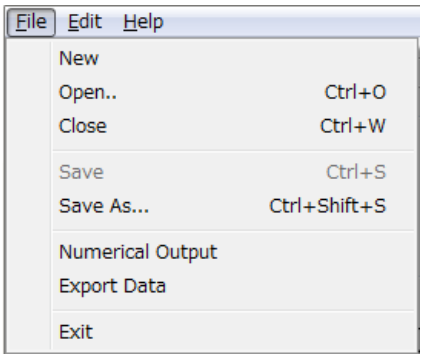
   Indexes of reflections you want to check will be specified in a column (up to 9 reflections). Reflections in each column will be displayed graphically in the same page (up to 10 pages).

   Reflection indexes should be specified by a two-dimensional index in a

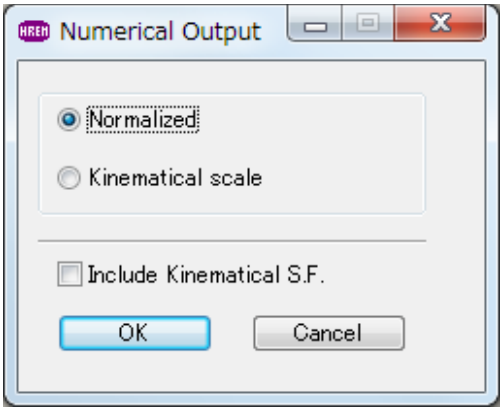
(projected) diffraction pattern.

Output Diffraction Intensity

Choose “Numerical Output” in File menu to view diffraction intensity (amplitude and phase) in numerical value.



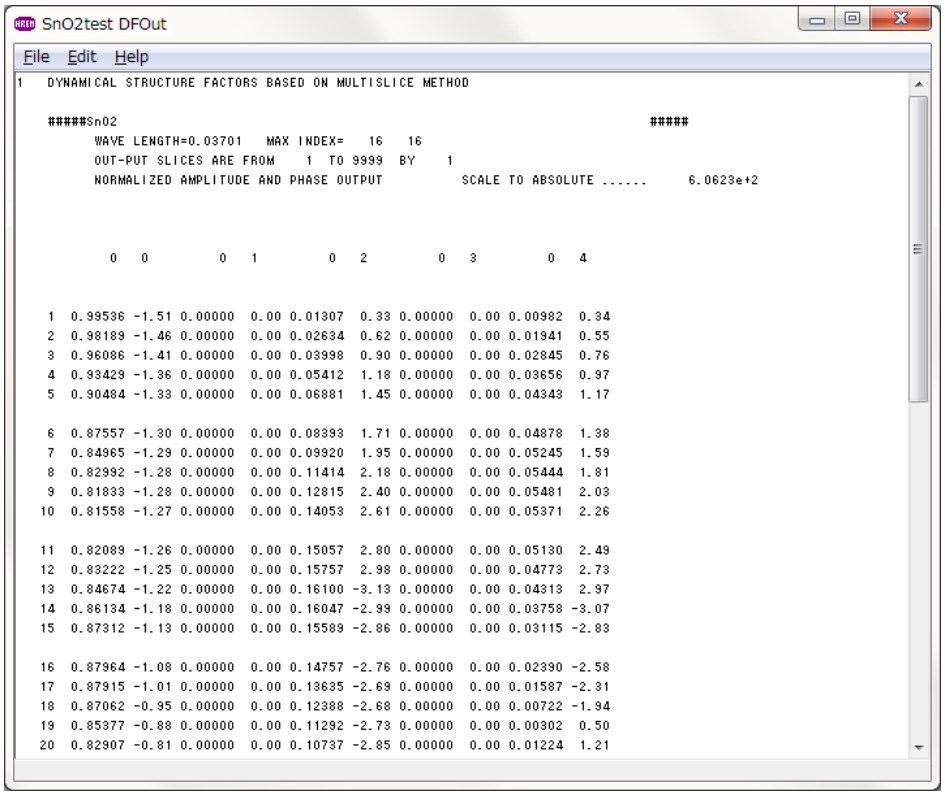
Then, the dialog “Numerical Output” for output control will appear.



The amplitude is displayed as a normalized value relative to an incident wave (Normalized), or as a scaled value relative to kinematical scattering amplitude (Kinematical scale).

If the checkbox “Include Kinematical S.F.” is selected, the kinematical structure factor will be included at the top of the numerical output.

Clicking “OK” button, the separate windows will be open, where amplitudes and phases of the specified reflections are displayed numerically. When an execution terminates normally, you will see the message "Execution completed. Congratulations!"



TIPS: The kinematical structure factors (scattering amplitudes) used in potential calculation will be displayed, when you check the “Include Kinematical S.F.” check box, or set a starting slice to zero in “Output Range” section.

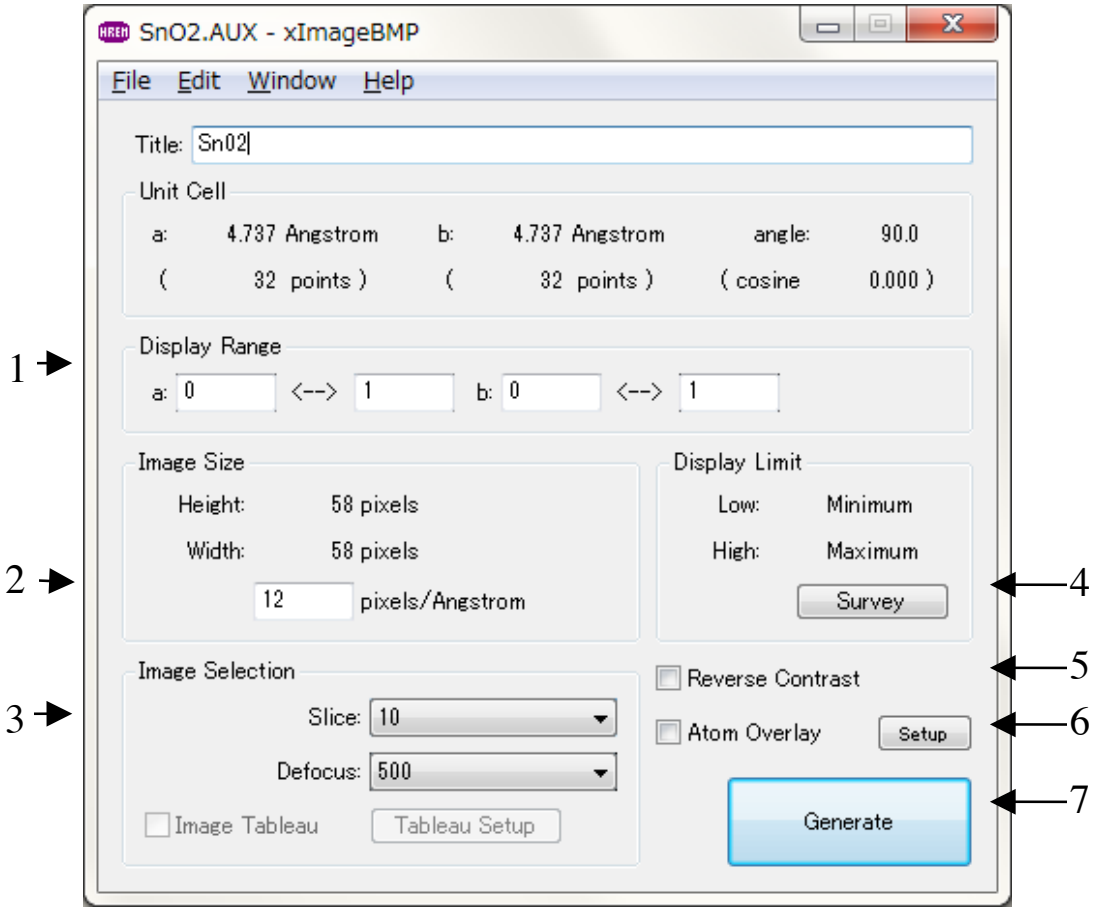
NOTE: The progress window has the fundamental menus such as File and Edit, and you can Save the content of the window from the File menu.

TIPS: The program can be terminated even in the middle of calculation by Exit command from the File menu or clicking the close button.

■ ImageBMP Reference

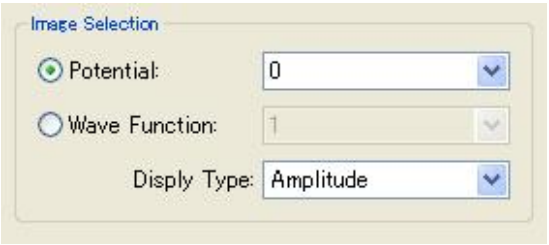
WORKSHEET

For EM Image Intensity Data



The title of the data and its projected two-dimensional cells (and the number of sampling points) will be shown at the top part of the window.

For Data from Dynamical Scattering Calculation



For EM Image Intensity Data

1. Display Range

   The range of display will be defined in terms of unit cell.

2. Scale (pixel/Angstrom)

   The scale will be specified by a number of pixels per Angstrom. Total numbers of pixels (Height and Width) to be displayed will be shown estimated according to the scale.

3. Image Selection

   - Slice

     The specimen thickness (slice number) for an EM image to be displayed will be selected from the slice list. When you select "All", images for all slices in the list will be generated one by one. When you choose “Select”, a dialog where you can select individual image will appear.

   - Defocus

     The defocus value for an EM image to be displayed will be selected from the defocus list. When you select "All", images for all defocus values in the list will be generated one by one. When you choose “Select”, a dialog where you can select individual image will appear.

   NOTE: In this utility an *under-focus* value is always *positive* irrespective of your defocus sign selection in the "Preferences."

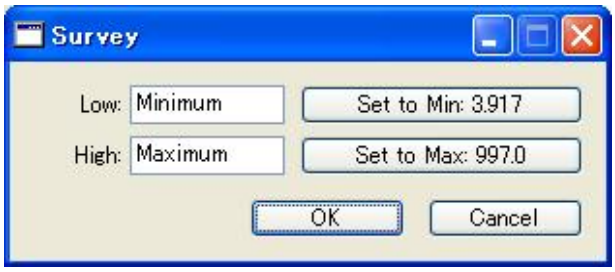
   - Image Tableau (Table Layout)

     This will control the way of display of selected images. When checked, the selected images will be displayed in a table layout. Otherwise, each selected images will de displayed separately. When you click “Tableau Setup” button, a dialog to setup a layout will be opened.

4. Survey

   Clicking "Survey" will open a small window showing a display range

(Maximum and minimum values).



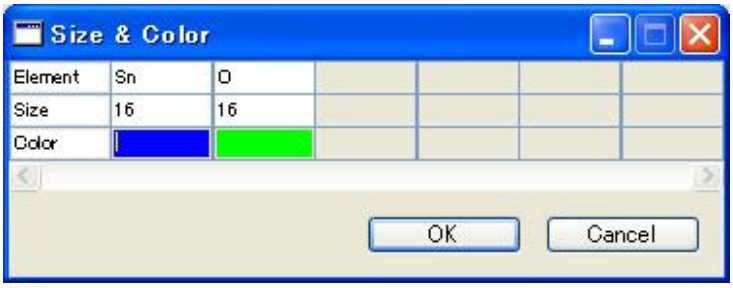
You can change the display ranges by setting numbers in the boxes.

5. Reverse Contrast

   When checked, the image will be displayed with a reversed contrast.

6. Atom Overlay

   When checked, a colored circle will be drawn on each atom position. The size and color of circle for each element will be changed in the dialog that will appear when you click “Setup” button.



7. Generate

   Gray scale image will be generated by clicking "Generate."

For Data from Dynamical Scattering Calculation

In the selection you can choose either "Potential" of "Wave Function" to be displayed as a gray scale image.

- Potential

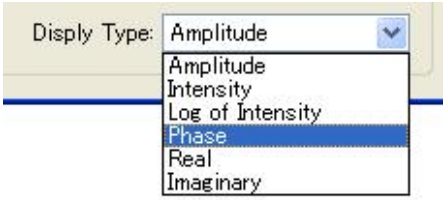
  The phase grating number (slice number) for which a potential distribution is displayed will be selected from the phase grating list. When you select "All", the potential distributions for all phase gratings in the list will be generated one by one. When you select "Projection", an image obtained by summing the potentials over all slices will be displayed.

- Wave Function

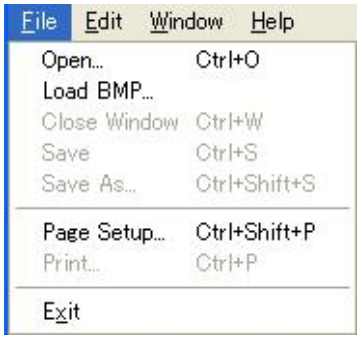
  The specimen thickness (slice number) at which a wave function is displayed will be selected from the slice list. When you select "All", images of all wave functions in the list will be generated one by one.

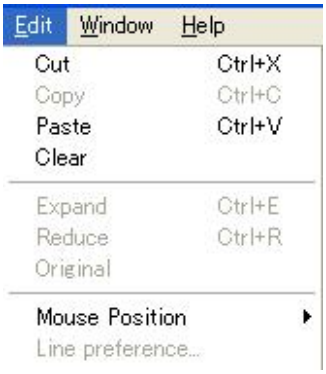
- Show

  As the potential and wave-function are saved in complex number, you have to choose a quantity to be displayed as a gray scale image from a following list:



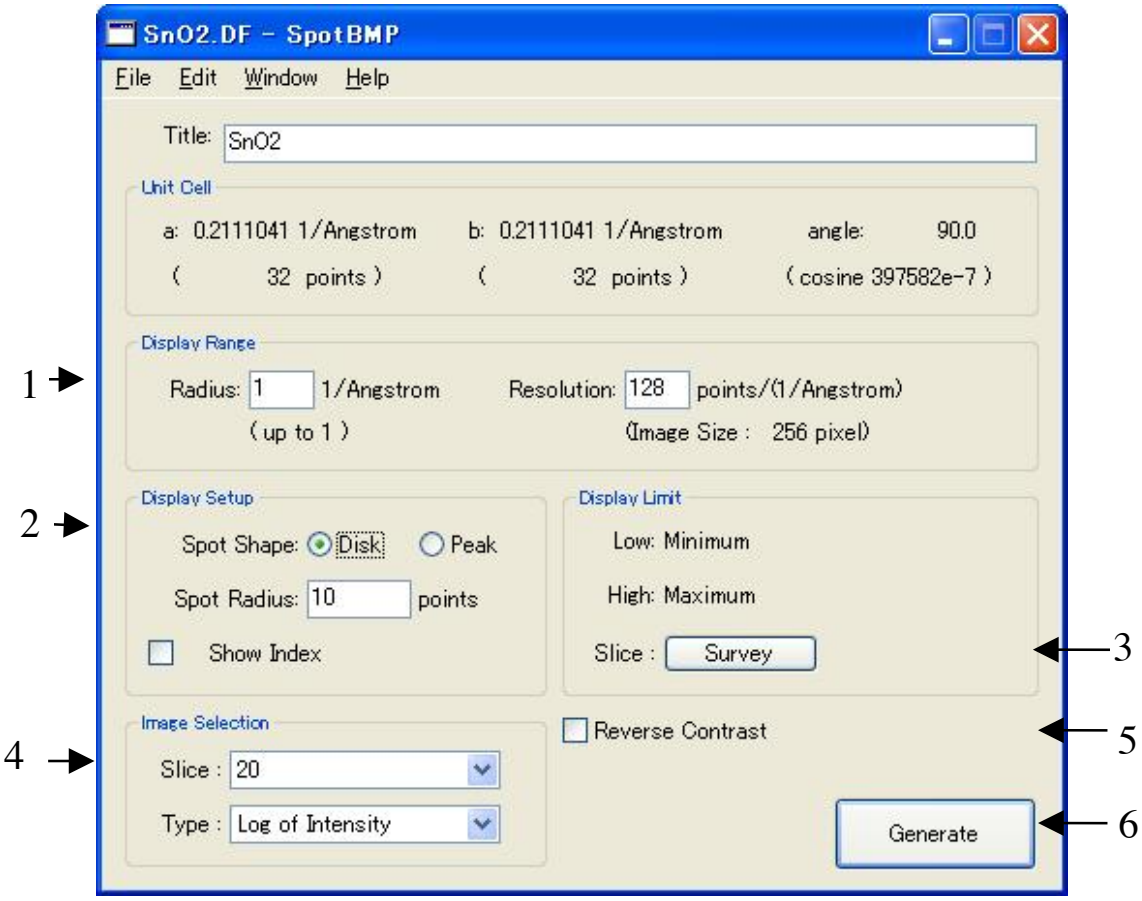
ImageBMP Menu





■ SpotBMP Reference

WORKSHEET



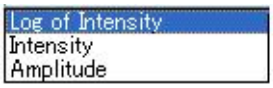
The title of the data and its projected two-dimensional cells (and the number of sampling points) will be shown at the top part of the window.

1. Display Range
   - Radius

     The diffraction area to be displayed will be specified by its radius (in 1/Angstrom) from the center. The displayable area that is outputted by the dynamical calculation program is indicated below the box.
   - Resolution

     The resolution will be specified by a number of pixels per 1/Angstrom. An image size to be displayed will be shown estimated according to the resolution.
2. Display setup

- Type



  Display data type will be selected from the following list:

- Show Index

  On/off the reflection index display on the gray scale image

- Spot shape

  You can choose a display shape of reflection spots from either "Dusk" or "Peak."

- Spot radius

  Size of each diffraction spot in pixels.

- Background Color

  "White" background displays an image like a negative, and "Black" background emulates an output on a printing paper.

3. Survey

   Clicking "Survey" will open a small window showing a display range (Maximum and minimum values).

   You can change the display ranges by setting numbers in the boxes.

4. Slice

   The specimen thickness (slice number) at which a diffraction pattern is displayed will be selected from the slice list. When you select "All", images of all diffraction patterns in the list will be generated one by one.

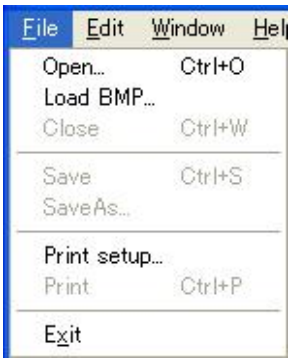
5. Reverse Contrast

   When checked, the image will be displayed with a reversed contrast.

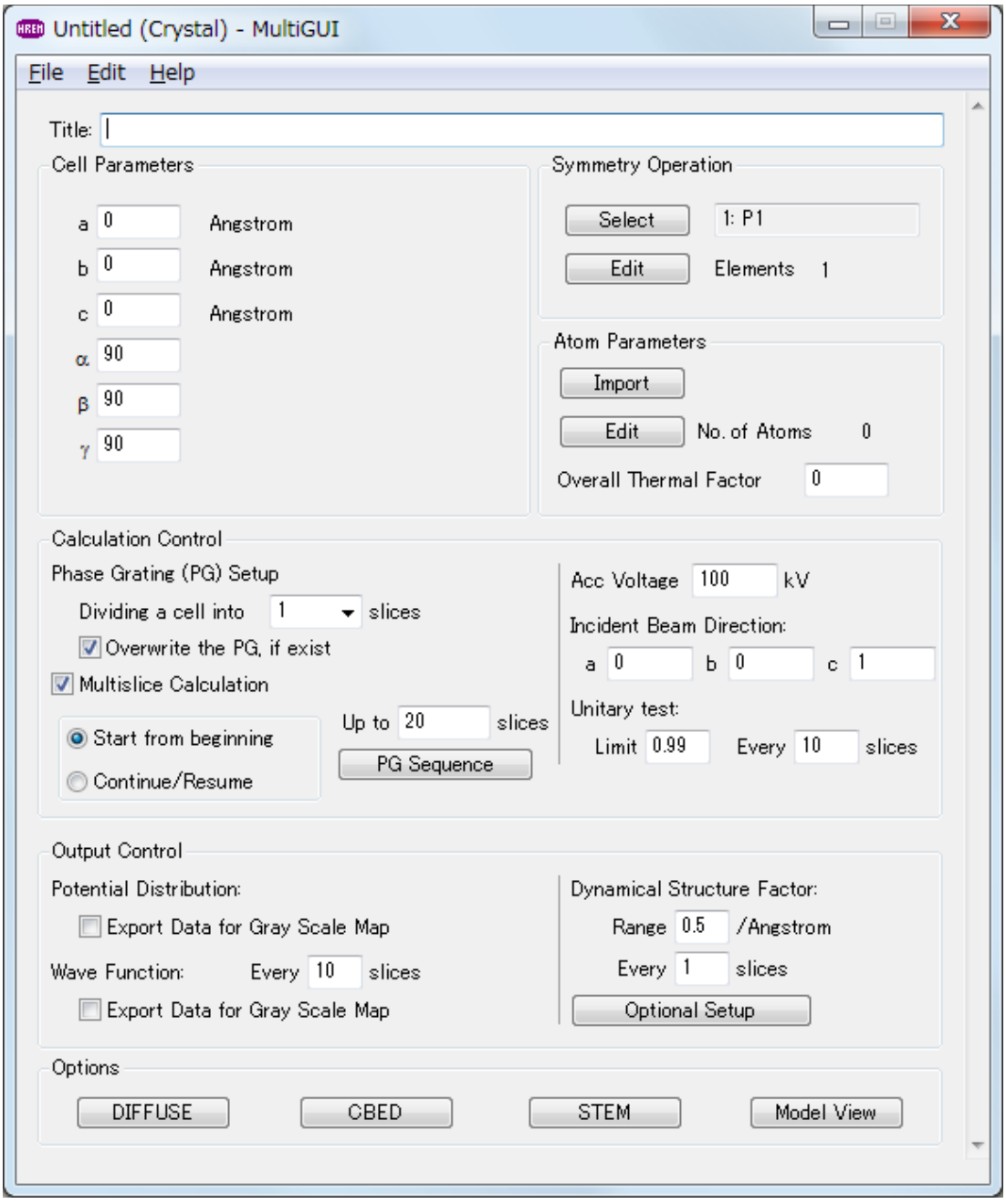
6. Generate

   Gray scale image will be generated by clicking "Generate."

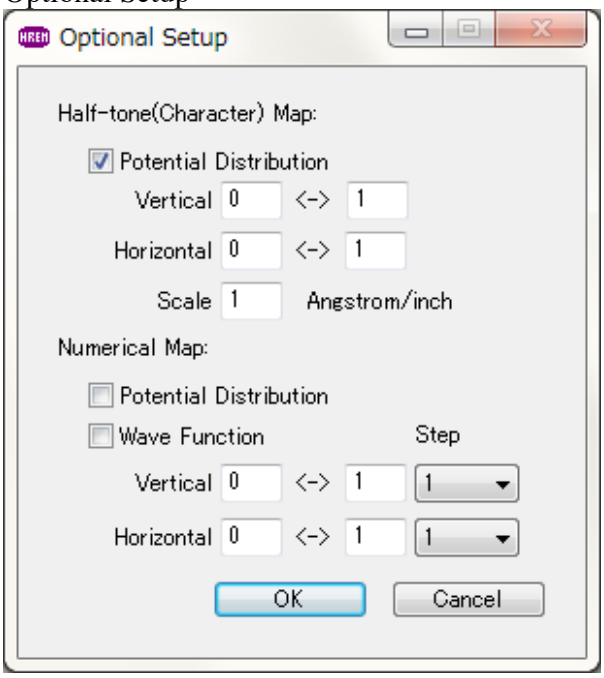
SpotBMP Menu

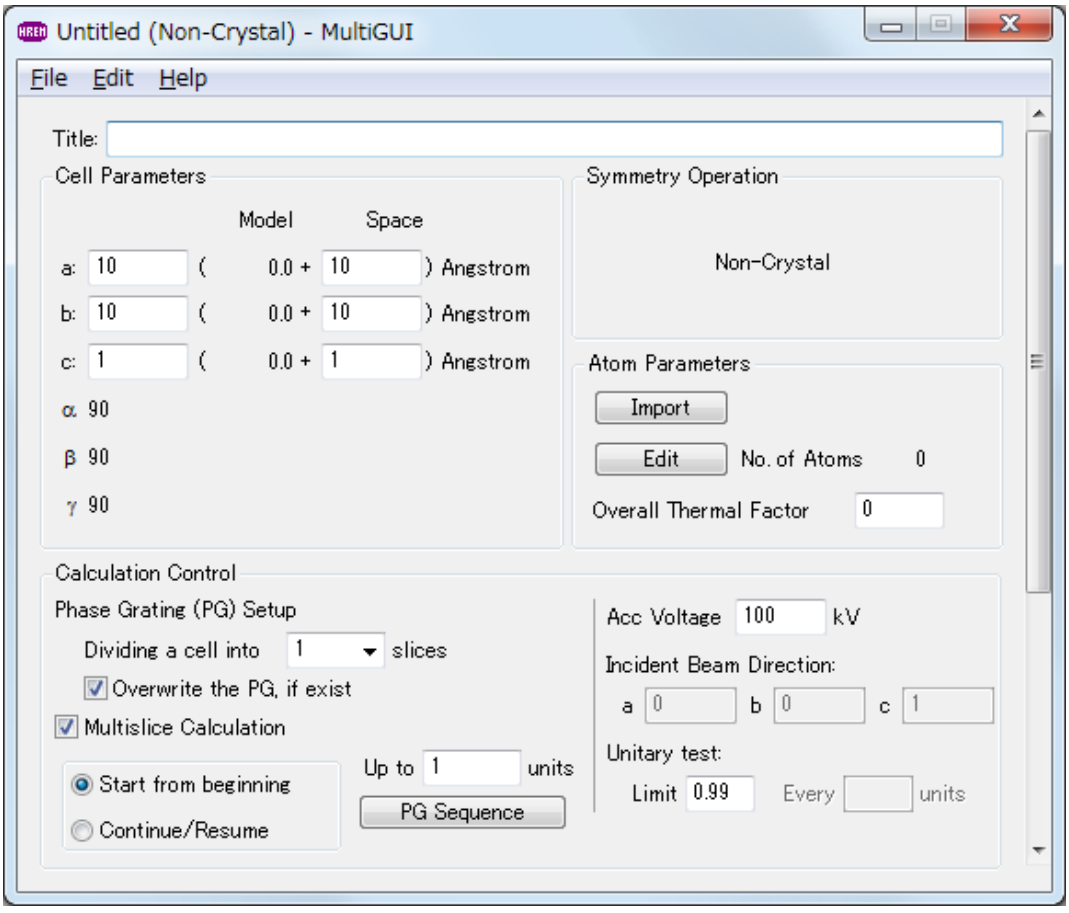


MultiGUI

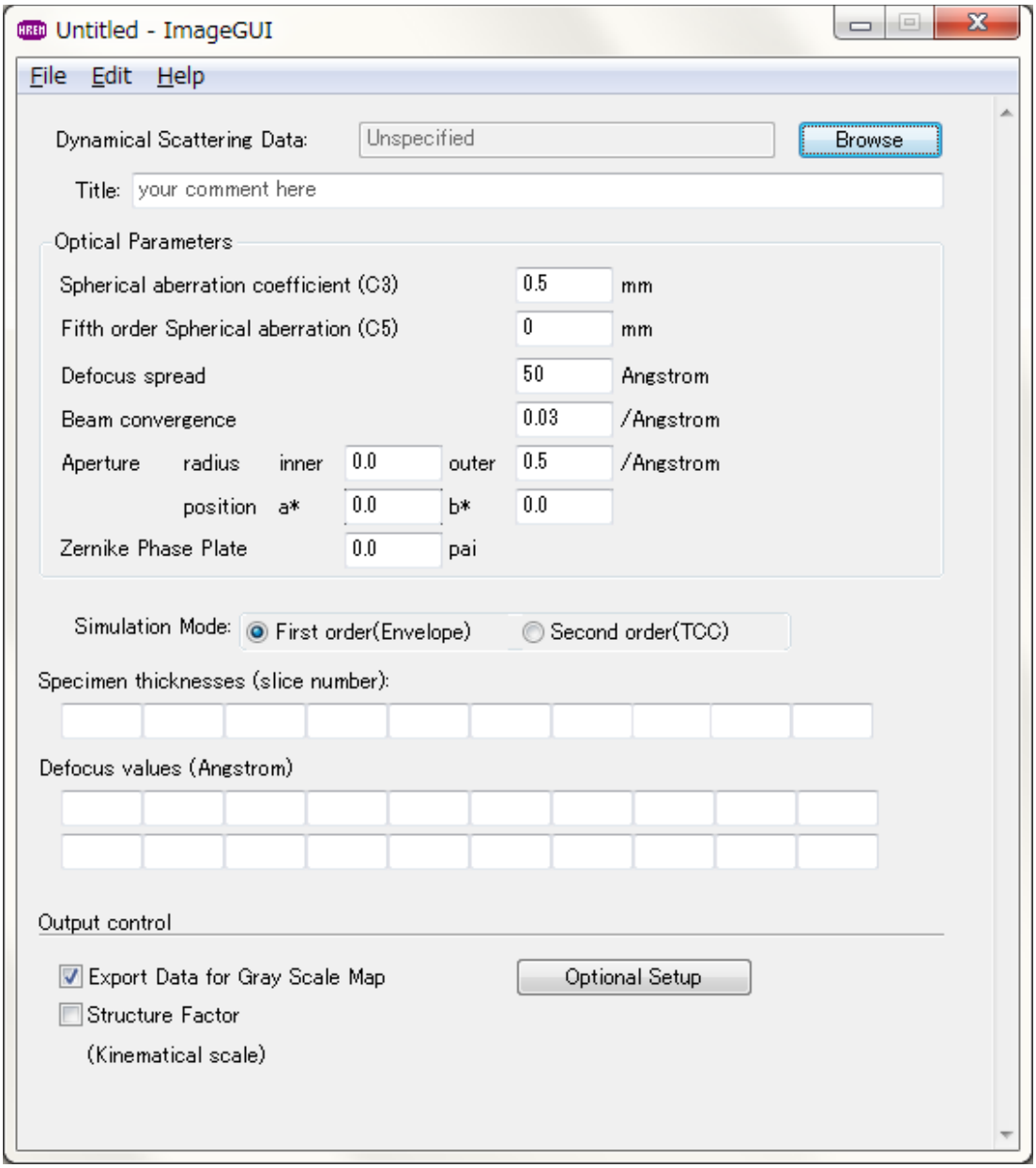

Untitled (Crystal) - MultiGUI
File Edit Help
Title:
Cell Parameters
a 0 Angstrom
b 0 Angstrom
c 0 Angstrom
α 90
β 90
γ 90
Symmetry Operation
Select 1: P1
Edit Elements 1
Atom Parameters
Import
Edit No. of Atoms 0
Overall Thermal Factor 0
Calculation Control
Phase Grating (PG) Setup
Dividing a cell into 1 slices
Overwrite the PG, if exist
Multislice Calculation
Start from beginning
Continue/Resume
Up to 20 slices
PG Sequence
Acc Voltage 100 kV
Incident Beam Direction:
a 0 b 0 c 1
Unitary test:
Limit 0.99 Every 10 slices
Output Control
Potential Distribution:
Export Data for Gray Scale Map
Wave Function: Every 10 slices
Export Data for Gray Scale Map
Dynamical Structure Factor:
Range 0.5 /Angstrom
Every 1 slices
Optional Setup
Options
DIFFUSE
CBED
STEM
Model View

Optional Setup

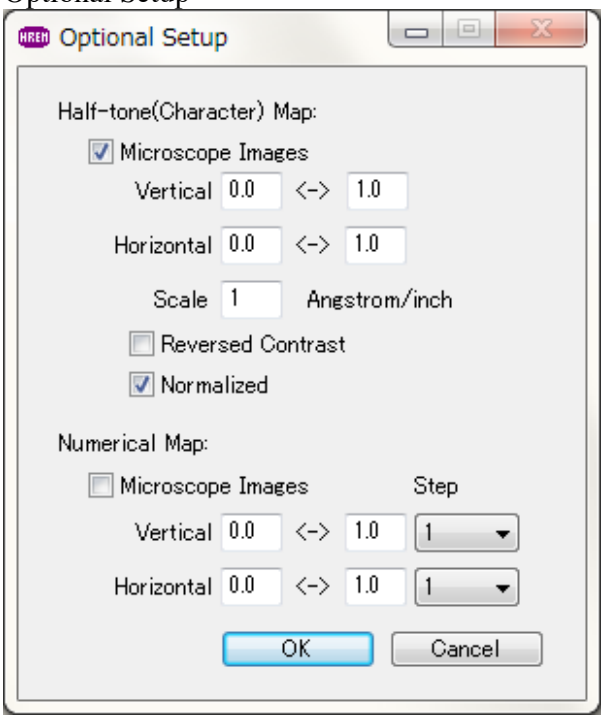




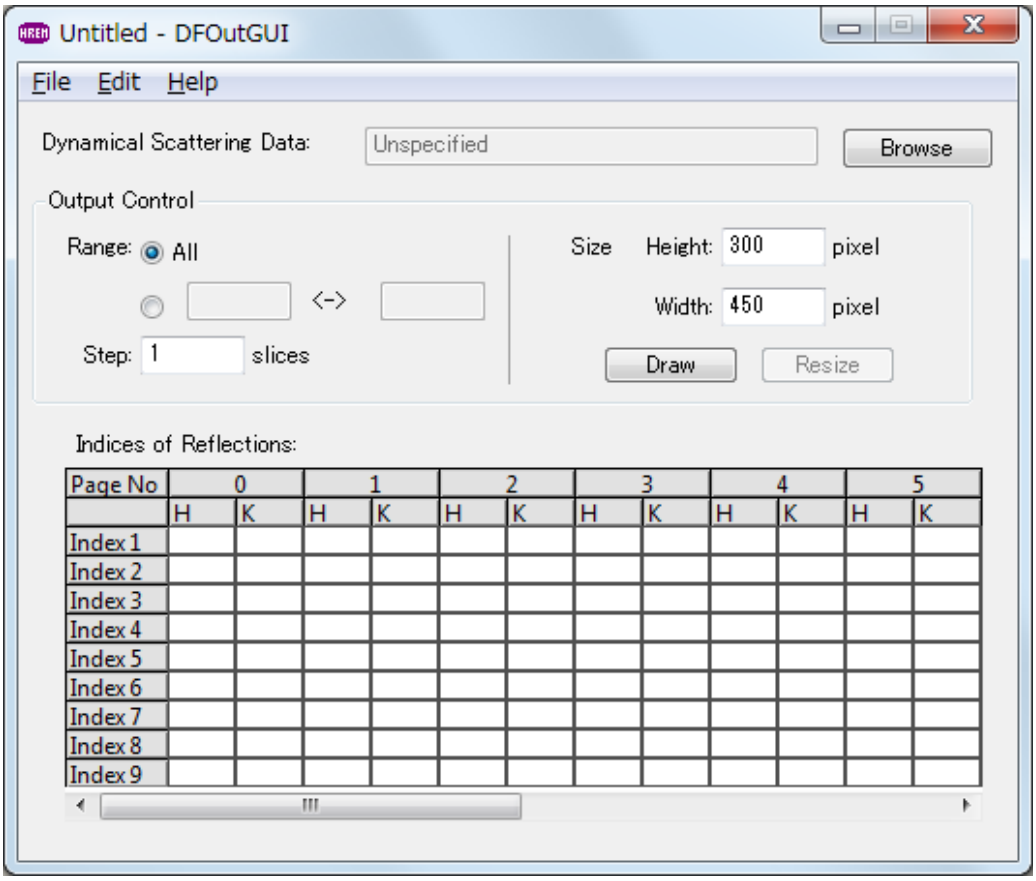
ImageGUI


Untitled - ImageGUI
File Edit Help
Dynamical Scattering Data:
Unspecified
Browse
Title:
your comment here
Optical Parameters
Spherical aberration coefficient (C3)
0.5
mm
Fifth order Spherical aberration (C5)
0
mm
Defocus spread
50
Angstrom
Beam convergence
0.03
/Angstrom
Aperture radius inner
0.0
outer
0.5
/Angstrom
position a*
0.0
b*
0.0
Zernike Phase Plate
0.0
pai
Simulation Mode:
First order(Envelope)
Second order(TCC)
Specimen thicknesses (slice number):
Defocus values (Angstrom)
Output control
Export Data for Gray Scale Map
Optional Setup
Structure Factor
(Kinematical scale)

Optional Setup



DFOutGUI


Untitled - DFOutGUI
File Edit Help
Dynamical Scattering Data:
Unspecified
Browse
Output Control
Range: All
<->
Step: 1 slices
Size Height: 300 pixel
Width: 450 pixel
Draw
Resize
Indices of Reflections:
Page No 0 1 2 3 4 5
H K H K H K H K H K H K
Index 1
Index 2
Index 3
Index 4
Index 5
Index 6
Index 7
Index 8
Index 9

FAQ

Frequently Asked Questions

This chapter will answer to Frequently Asked Questions with Q&A style

Dynamical Scattering Calculation（MultiGUI）

Q001: How to use Atom Parameter Editor?

Q002: How to use ”Occupancy”?

Q003: I saw the example, where an angle of lattice parameter is zero (o)…

Q004: How many phase gratings can we use?

Q005: How many slices can we divide a unit cell (or a super-cell) into?

Q006: How is a phase grating (transmission function) evaluated?

Q007: How to specify the range of scattered waves to be included in the multislice calculation?

Q008: What is a slice thickness for [011] or [111] incidence?

Q009: How to specify an incident beam direction?

Q010: Why is the incident beam direction with c=0 not allowed?

Q011: How to treat an incident beam direction with c=0?

Q012: How is an atom scattering factor for electrons calculated?

Q013: Can we use scatter factor for ions?

Q014: How to specify a thermal factor (thermal vibration effect)?

Q015: How does thermal factor affect an atomic scattering factor?

Q016: How do we use “Unitary test”?

Q017: What kind of propagation function is used in calculation?

Q018: What is three-dimensional effect?

Q019: How to include three-dimensional effect in multislice calculation?

Q020: How to specify model symmetry (symmetry operations)?

Q021: I can’t read atom parameters from a text file.

Q022: How to create an atom parameter file (text data)?

Q023: What is a format of atom parameter file (test data)?

Q024: How does an atomic potential contribute to a projected potential?

Image Calculation（ImageGUI）

Q101: My image does not show any contrast.

Q102: Let me know the differences between Simulation Modes.

Q103: When I select “First Order (Envelope)” from Simulation Mode, I can get a correct image, but not with “Second order (TCC)”.

Dynamical Scattering Amplitude Output（DFOutGUI）

Q201: Why is a reflection specified using only two indexes? How can we relate these indexes to a normal three-index system?

Q202: How is the phase displayed?

CBED Extension

Q301: High angle area is not displayed.

Q302: Does HOLZ lines appear under the projection approximation?

Q303: Can we calculate a Large-angle CBED (LACBED, Tanaka pattern)?

Q304: How can we improve HOLZ line accuracy?

STEM Extension

Q401: An output from STEM image does not seem to represent a model structure

Q402: How to select a super-cell size?

Q403: Computation becomes extremely slow, when a model size becomes large.

Q404: What is a range to be included for scattering calculation? Does this range depend on the model size?

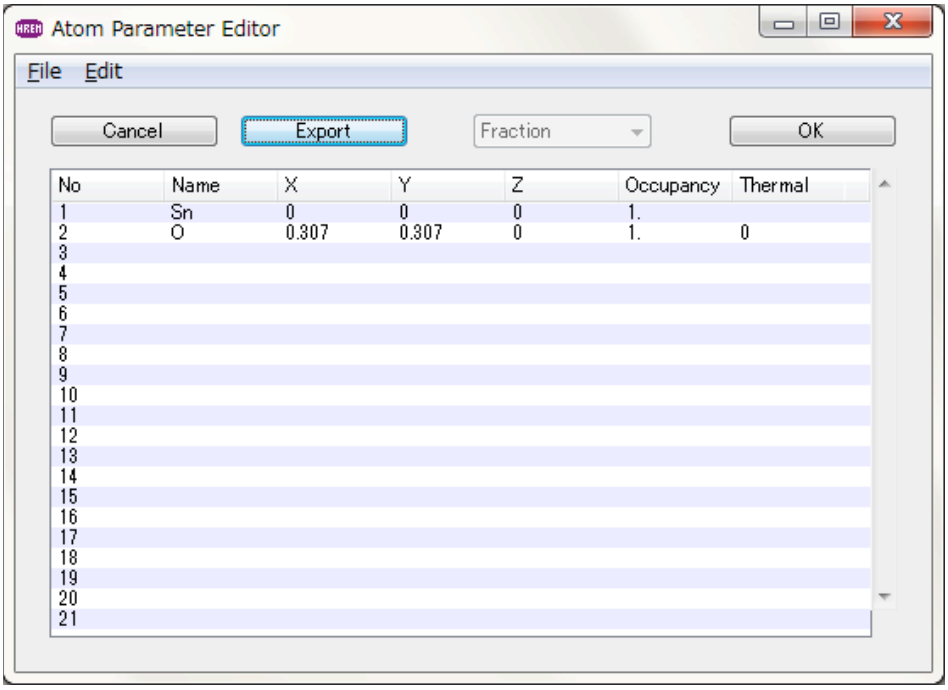
Q405: What is a strategy to shorten computation time?

Dynamical Scattering Calculation（MultiGUI）

Q001 How to use Atom Parameter Editor?

A

1. Click “Edit” button from Atom Parameters pane. Then, the following “Atom Parameter Editor” window will appear. In this example, the parameters for two atoms are already registered.



2. Input the following parameters for each atom in separate row.
   - “Name”: Atom identifier including an element name. You can add figure(s) before or after the element name to identify each atom.
   - “x”, “y” and “z”: Atom positions in terms of a unit cell length.
   - “Occupancy”: Average probability of occupying the site (normally one).
   - “Thermal”: Thermal parameter, namely Debye-Waller factor. If this parameter is zero (0), “Overall Thermal Factor” will be used.
3. When you finish entering the parameters for all the atoms, click “OK” to save the data and close the window. You can click “Cancel” to abort an input at any time.

NOTE You can save atom parameters as a text file by clicking “Export.” Then, you can edit its content easily using your favorite text editor. You can import atom parameters in a text file using “Import” in the “Atom Parameters” pane of MultiGUI. Please check also Q023.

Q002 How to use ”Occupancy”?

A "Occupancy" is a probability, with which the element occupy the site as an average over many unit cells. Since each element cannot occupy the site in fraction, occupancy is normally one (1). However, in a disordered structure, for example, a specific site will be occupied more than one element, and an occupancy of each element becomes less than one,

For a special atom position, the symmetry operation generates an atom at the original atom position. "Multiplicity" (the total number of symmetry-generated atoms at the same position) is automatically taken into account by xHREM, so you may not necessary to set "Occupancy" to 1/"Multiplicity" as sometime required by other software.

Q003

I saw the example, where an angle of lattice parameter is zero (o)…

A You can specify an angle in terms of cosine. Thus, zero means 90 degree. However, you should not mix a degree and cosine, so a mixed set of three angles, say 0, 0, 120 are not acceptable.

TIPS Cosine of the angle is used inside the program.

Q004

How many phase gratings can we use?

A You can use up to 1000 different phase gratings. The sequence of the phase grating to be used in calculation will be easily is specified by using "PG Sequence Editor".

Q005

How many slices can we divide a unit cell (or a super-cell) into?

A Since the maximum different phase grating is 1000, you can divide the unit cell (your model structure) into 1000 slices.

Q006

How is a phase grating (transmission function) evaluated?

A A phase grating is directly evaluated by assigning a projected potential of the slice to a complex exponential function. Here, the direction of potential projection is not perpendicular to the slice, but along the incident beam direction.

Q007

How to specify the range of scattered waves to be included in the multislice calculation?

A The range of scattered waves included in the multislice iteration is specified by "Range" parameter of "Dynamical Calculation" pane of the Preferences window.

Q008 What is a slice thickness for [011] or [111] incidence?

A Normally, the slice thickness is measured perpendicular to the slice (this is a physical thickness of the slice). However, the length of a slice measured along the incident beam direction is more important from electron scattering point of view.

For example, the scattering conditions are different even for the same incident beam direction of [011], when the incident surfaces is (001) or (011). xHREM can handle such differences.

xHREM uses the slice that is always parallel to the entrance surface, but projects the potential along the incident beam direction.

If you are interested in knowing more details, please consult the paper:
K. Ishizuka, *Acta Cryst.* A38 (1982) 773-779.

Q009 How to specify an incident beam direction?

A An incident beam direction $\boldsymbol{t}$ is specified by three unit cell vectors in the real space as follows: $\boldsymbol{t} = d_1\boldsymbol{a} + d_2\boldsymbol{b} + d_3\boldsymbol{c}$

For example, the incident beam direction parallel to c-axis is defined as [0, 0, 1]. If the incident beam direction is not specified by a simple sum of three unit cell vectors, it is not a good condition to take an EM image.

NOTE In an experiment of electron diffraction, the incident beam direction may be specified by the Laue point, which corresponds to the Ewald sphere center projected on the observation diffraction plane.

TIPS Given the incident beam directions specified in real and reciprocal unit cell

$$\begin{aligned}\boldsymbol{t} &= \mathrm{d}_1\boldsymbol{a} + \mathrm{d}_2\boldsymbol{b} + \mathrm{d}_3\boldsymbol{c} \\ &= \mathrm{r}_1\boldsymbol{a}^* + \mathrm{r}_2\boldsymbol{b}^* + \mathrm{r}_3\boldsymbol{c}^*\end{aligned}$$

each coefficient can be easily evaluated as follows:

$$d_1 = \boldsymbol{t}\boldsymbol{a}^* = r_1 a^{*2} + r_2\boldsymbol{b}^*\boldsymbol{a}^* + r_3\boldsymbol{c}^*\boldsymbol{a}^*$$

$$r_1 = \boldsymbol{t}\boldsymbol{a} = d_1 a^2 + d_2\boldsymbol{b}\boldsymbol{a} + d_3\boldsymbol{c}\boldsymbol{a}$$

Q010 Why is the incident beam direction with c=0 not allowed?

A xHREM assumes that an incident surface is the (001) plane (the c-plane of an input unit cell). Thus, the incident beam direction with c=0 means that the electron beam is parallel to an entrance surface, which is not occurred in practice.

TIPS You can specify an incident surface of the specimen, on which an electron beam impinges. Therefore, using xHREM it may become possible to treat a surface effect that is usually neglected by other programs.

Q011 How to treat an incident beam direction with c=0?

A An incident beam direction with c=0 in terms of an input unit cell is not accepted (see Q010). To handle this problem, you can transform the coordinate system from "Preferences" dialog under Edit menu, and make the entrance surface include the c-axis.

MultiGUI takes care of all the necessary transformations, such as atomic coordinates, symmetry operations, an incident beam direction and so on, and creates a correct data set for calculation.

Q012 How is an atom scattering factor for electrons calculated?

A Atom scattering factor (ASF) can be chosen from the following two types in the "Atom Scattering Factor" pane of "Preferences".

Doyle-Turner: ASF for electrons is calculated from x-ray ASF using the following Mott's formula:

$$f_e(s) = 0.023934\left\{Z - f_x(s)\right\}/s^2; \quad s = \sin\theta/\lambda$$

Here, x-ray ASF is approximated by a sum of Gaussians, whose coefficients are tabulated in *International Tables for x-ray Crystallography*, Vol. IV. It should be noted that Doyle-Turner ASF is valid only up to s=2.0.

Weikenmeier-Kohl: This form factor is valid also for high-angle scattering beyond s=2.0. Thus, this form factor can be used to estimate absorption potential due to thermal diffuse scattering (TDS).

Q013 Can we use scatter factor for ions?

A In principle, the answer is YES. However, the current GUI does not support such cases, and you have to modify manually the data (.DA1) created by MultuGUI. Please contact our user support for detailed steps.

Q014 How to specify a thermal factor (thermal vibration effect)?

A Effect of thermal vibration is taken into account by using a Debye-Waller thermal factor.

- When you want to use a different thermal factor to each atom, you can specify each thermal factor at "Thermal" column of atom parameters.
- When "Thermal" parameter of individual atom is zero, the thermal factor specified at "Overall Thermal Factor" will be applied to that atom,

TIPS For simplicity, you may want to use the same thermal factor for all the atoms in the model. In this case, specify the thermal factor in "Overall Thermal Factor" and leave blank (or set to zero) at "Thermal" column of each atom.

Q015 How does thermal factor affect an atomic scattering factor?

A An atomic scattering factor (ASF) is attenuated by a Debye-Waller thermal factor B as a function of a scattering angle θ:

$$\exp\left\{-B\left(\frac{\sin\theta}{\lambda}\right)^2\right\}$$

You may note that high-angle scattering is more affected by thermal vibration than low-angle scattering.

Q016 How do we use "Unitary test"?

A Without absorption there is no decrease of electrons. Thus, the total sum of electron density distribution or electron diffraction distribution is always constant. However, if an enough scattering area is not included in scattering calculation, some electrons tends to scatter outside of the scattering area, and the total sum of diffracted electrons will decrease with a sample thickness. Therefore, Australian group introduced the Unitary Test to check calculation conditions for their reciprocal-space multislice formula.

However, xHREM uses the multislice formula (in mixed-space) based on Fast Fourier Transform (FFT), and thus the total sums of both electron density distribution and electron diffraction distribution are identical, and always equal to unity. Therefore, a usual way of Unitary Test has no meaning.

The Unitary Test of xHREM calculates the total sum of electron diffraction distribution excluding intensities at the outermost pixels. Therefore, if an enough scattering area is not included in scattering calculation, the total sum of scattering distribution will decrease with a sample thickness. However, since this attenuation is mild, the Limit of Unitary Test should be very close to one to make the test effective.

NOTE When you include absorption due to thermal diffuse scattering (TDS) using Weikenmeier-Kohl atomic scattering factors, a number of electrons will actually decrease due to absorption. Thus, if you don't set the Unitary Test limit sufficiently low, a computation will stop in the middle of multislice iteration (scattering calculation) owing to the Unitary Test.

Q017 What kind of propagation function is used in calculation?

A xHREM uses the propagation function that corresponds to a spherical wave, not a propagation function with parabola approximation. If you are interested in knowing more details, please consult the paper: K. Ishizuka, *Acta Cryst.* A38 (1982) 773-779.

Q018 What is three-dimensional effect?

A Three-dimensional effect is such that relative atom positions along the incident direction of an electron beam affect scattering intensity distribution,

Q019 How to include three-dimensional effect in multislice calculation?

A Three-dimensional effect may be included in multislice calculation, when relative atom positions along the incident direction of an electron beam are taken into account by dividing a unit cell (model structure) into a multiple slices.

NOTE How accurate the multislice formulation can take into account a three-dimensional effect is still an open question.

Q020 How to specify model symmetry (symmetry operations)?

A The way to specify symmetry operations follows the rule used in *International Tables for Crystallography*.

- yxz components of symmetry operation will be separated by a comma (,).
- each symmetry operation will be separated by a semicolon (;).
- end of all the symmetry operation is a period (.).

Example:
x, y, z; y, x, z+1/2.

Q021 I can't read atom parameters from a text file.

A Please make sure that you are specifying parameter entries in a correct order.

Q022 How to create an atom parameter file (text data)?

A Input a name, coordinates (x, y, z), occupancy and thermal factor for each atom in a single line using an editor or a word processor. A serial number can be added at the beginning of each line. Each parameter will be separated by a comma (,) or any number of spaces (blanks). Thus, you don't need to align the column position of each parameter.

Example

Name	X	Y	X	Occupancy	Thermal
Sn1	0	0	0	1.0	0
O1	0.307	0.307	0	1.0	0

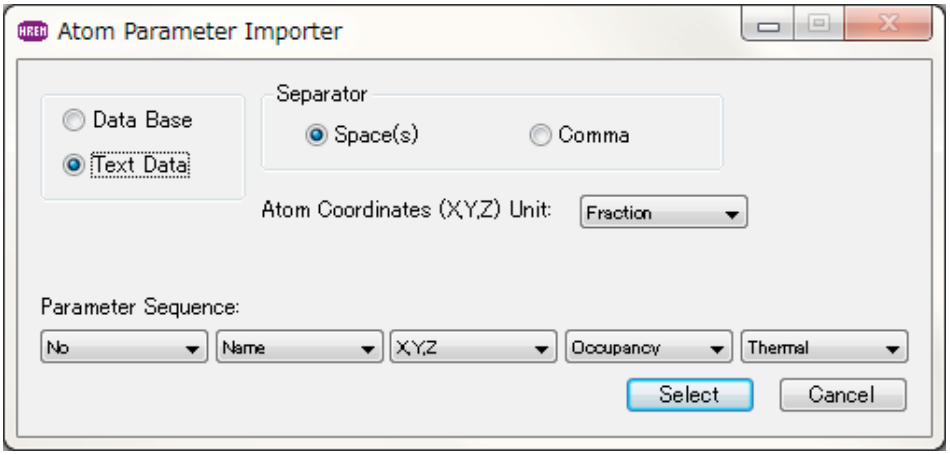
NOTE Name should include an element name. You can add a number to the element name to distinguish different atoms of the same element.

Save a created data to a text file (sample-name.atm).

Q023 What is a format of atom parameter file (test data)?

A Atom parameter file is a text file, each line of which contains a name, coordinates (x, y, z), occupancy and thermal factor. A number can be added at the beginning of each line. Each parameter will be separated by a comma (,) or any number of spaces (blanks). Thus, you don't need to align the column position of each parameter.

The order of parameters in the text file may be arbitrary, since the order of parameters can be specified as shown below, when you read them.



Unit of the atom coordinates can be selected using Atom Coordinates Unit pull-down. This function is especially useful, when you create a atomic model using a third-party model building application.

Q024 How does an atomic potential contribute to a projected potential?

A When a whole unit cell is treated as a single slice (projection approximation), a whole atomic potential will be projected.

When a unit cell is divided into a multiple slices, in principle, only the part of potential belongs to a slice should be projected. However, xHREM will project the whole atomic potential to the slice, which the center of atom (atom coordinate) belongs to. In this way, we can use the projection theorem of Fourier transform to efficiently project an atom potential.

Image Calculation（ImageGUI）

Q101 My image does not show any contrast.

A Please check an aperture radius for image calculation. The smallest fringe spacing that will contribute to image formation depends on the unit (s or d*), which you can select from “Preferences” window. (Note: 2s = d*)

The smallest fringe spacing = 1/2s = 1/d*

Especially, when you have forbidden reflections, please check whether allowed reflections are included within the aperture.

Q102 Let me know the differences between Simulation Modes.

A Simulation Mode determines the way to treat partial coherence.

Using xHREM you can choose a commonly used technique using Envelope functions, or a more elaborate technique using Transmission Cross-coefficient (TCC).

The technique using TCC, except a small model, requires more computation time than the technique using Envelope functions.

Q103 When I select “First Order (Envelope)” from Simulation Mode, I can get a correct image, but not with “Second order (TCC)”.

A In the case of “Second order (TCC)” the spatial frequencies of twice of the objective aperture radius will be included in image calculation. This is because interference terms between scattered waves that pass the objective aperture should be included in image calculation.

Thus, “Second order (TCC)” calculation requires the Fourier space that is twice of the aperture size, although “First Order (Envelope)” calculation requires the Fourier space that corresponds to the aperture size. Here, image calculation uses the same area (the same size of Fourier space) used by scattering calculation.

When the Fourier space used for image calculation is not enough, “Range” parameter of “Dynamical calculation” pane should be increased from the “Preferences” window of MultiGUI, and scattering calculation should be done again. The Fourier space used for image calculation cannot be modified by changing “Range” from the “Preferences” window of ImageGUI.

Note Except you don’t specify an exceptionally small “Range” for scattering calculation, this situation will not occur.

Dynamical Scattering Amplitude Output（DFOutGUI）

Q201 Why is a reflection specified using only two indexes? How can we relate these indexes to a normal three-index system?

A Multislice calculation determines scattering amplitudes using two-dimensional slices (Phase Gratings). Thus, a wave function calculated is two-dimensional, and its Fourier transform is also two-dimensional. The two indexes specifies a reflection in 2D reciprocal space.

This 2D index can be converted to a normal 3D index by finding a relation between the 3D reciprocal lattice and the 2D reciprocal lattice. The same technique can be used to find a relation for Higher Order Laue Zone (HOLZ).

Q202 How is the phase displayed?

A All the phases are shifted by $-\pi/2$, and thus the phase of scattered wave from a thin sample corresponds to the phase of crystallographic structure factor (the phase of the incident wave is displayed as $-\pi/2$).

In crystallography the phase of structure factor is zero or π for the structure that has a center of symmetry (Namely, the structure factor is real, and will be positive or negative value). xHREM makes the phase of scattered wave from a thin sample correspond to the phase of crystallographic structure factor.

CBED Extension

Q301 High angle area is not displayed.

A The output range of CBED pattern is specified by “Range” of “Dynamical Structure Factor” in “Output Control” pane. Please check the unit (s ot d*) and the specified output value.

Q302 Does HOLZ lines appear under the projection approximation?

A Yes, HOLZ lines will appear close to the correct positions even under the projection approximation. However, their intensities may not be accurate.

Q303 Can we calculate a Large-angle CBED (LACBED, Tanaka pattern)?

A In LACBED experiment, a sample is placed off the electron beam focus point. Then, only the transmitted beam selected by an aperture is recorded.

Since xHREM calculates a CBED pattern by creating the focused probe at the specimen entrance surface, LACBED cannot be obtained.

Q304 How can we improve HOLZ line accuracy?

A In order to get a fine HOLZ line, use a higher “Resolution” of “Calculation Control” of the CBED dialog. Please consult the CBED Manual for a calculation step for each resolution setting.

In order to obtain a CBED pattern with an accurate position and intensity of HOLZ lines, the 3D effect (see Q019) should be properly included. Thus, a unit cell should be divided into a multiple slices.

STEM Extension

Q401

An output from STEM image does not seem to represent a model structure.

A At first, check a projected model structure using Model Viewer (Model View of MultiGUI). If the projected model is displayed correctly, then check a scan step. If the scan step is larger than 0.3 A, you may not get a smoothed atomic structure.

NOTE: If a displayed projected model structure is not correct, even when input atom parameters and a selected space group are right, then the symmetry operations of the selected space group may be wrong. If you find such an error, please report your finding to our support.

Q402

How to select a super-cell size?

A The size of a super-cell determines a sampling interval of Fourier space (an inverse of super-cell size corresponds to a calculation step of scattering distribution). Therefore, a super-cell size of larger than 5 nm (scattering calculation step of less than 0.2 /nm) should be employed for a good simulation.

1. *Crystal model*

If a unit cell of the model is less than 5 nm, select "Standard" from "Super-cell size." Then, the input unit cell will be automatically repeated to create an approximately 5-nm super-cell. If a unit cell of the model is larger than 5 nm, select a size of super-cell larger than the unit cell.

2. *Interface or a defect model*

Select an appropriate size of super-cell that is larger than the longer edge of the structure model. Other short direction will be automatically repeated to fill the selected super-cell.

3. *Model with no periodicity, such as a nano-particle*

Select an appropriate size of super-cell that can accommodate the whole model.

Q403

Computation becomes extremely slow, when a model size becomes large.

A STEM calculation requires all the phase gratings at each scan point. Therefore, even when a part of phase gratings cannot be loaded into the mail memory (RAM), all the phase gratings should be read from an external memory for each scan points in the case of a large model. Since computation speed of a contemporary PC is astonishingly fast, a total computation time will be extremely deteriorated due to this data access.

To avoid this defect you have to install more RAM. If the total size of phase gratings becomes more than about 2GM, you may have to use the 64-bit version (*STEM Extension Pro*) that supports a 64-bit OS to handle more memory.

Q404 What is a range to be included for scattering calculation? Does this range depend on the model size?

A In order to evaluate probe propagation under elastic scattering, calculation including s=2.5/A (d*=5.0/A) is normally sufficient. This range does not depend on the model size.

Q405 What is a strategy to shorten computation time?

A Since STEM simulation requires scattering calculation at each scan point, a total computation time tends to become very long. The current version of STEM Extension supports Multi-CPU (core). Thus, if you use a PC with a multi-CPU, you can reduce a total computation time by a factor that is approximately a number of CPU (Core).

A further reduction of computation time will be obtained, if you use a cluster version (*STEM Extension Cluster*) that uses multiple computers simultaneously.